



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:47 AM UTC

PDB ID : 1Q3S / pdb\_00001q3s  
Title : Crystal structure of the chaperonin from Thermococcus strain KS-1 (FormIII crystal complexed with ADP)  
Authors : Shomura, Y.; Yoshida, T.; Iizuka, R.; Maruyama, T.; Yohda, M.; Miki, K.  
Deposited on : 2003-07-31  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

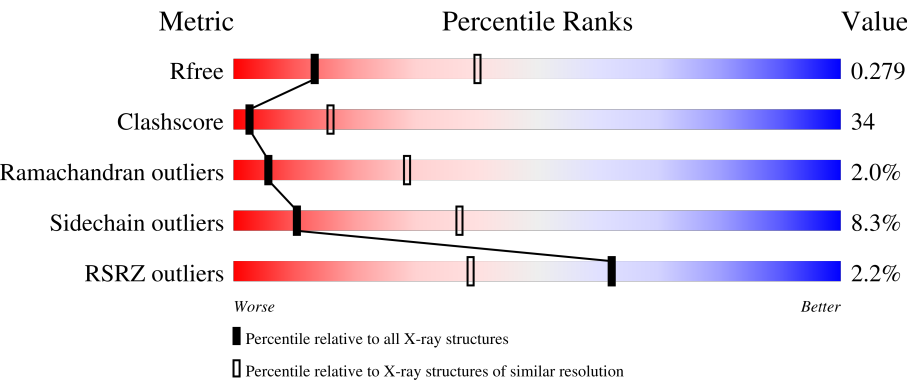
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2672 (3.00-3.00)                                      |
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 1   | A     | 548    | <div><div>2%</div><div>43%</div><div>44%</div><div>8%</div><div>6%</div></div> |
| 1   | B     | 548    | <div><div>2%</div><div>44%</div><div>44%</div><div>6%</div><div>6%</div></div> |
| 1   | C     | 548    | <div><div>2%</div><div>40%</div><div>48%</div><div>6%</div><div>6%</div></div> |
| 1   | D     | 548    | <div><div>2%</div><div>39%</div><div>47%</div><div>8%</div><div>6%</div></div> |
| 1   | E     | 548    | <div><div>2%</div><div>38%</div><div>49%</div><div>7%</div><div>6%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 548    |                  |
| 1   | G     | 548    |                  |
| 1   | H     | 548    |                  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31751 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thermosome alpha subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | B     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | C     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | D     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | E     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | F     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | G     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |
| 1   | H     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3941  | 2482 | 672 | 770 | 17 |         |         |       |

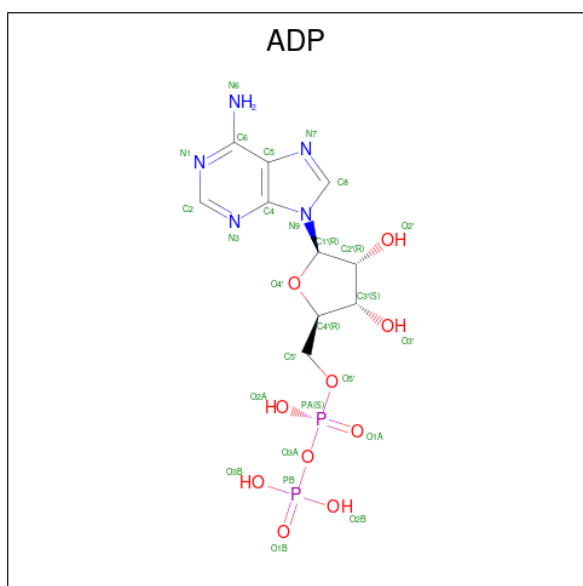
There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| B     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| C     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| D     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| E     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| F     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| G     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |
| H     | 65      | CYS      | GLY    | engineered mutation | UNP O24729 |

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 2   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 2   | C     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 2   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 2   | E     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 2   | G     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 2   | H     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 3   | A     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 3   | B     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 3   | C     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 3   | D     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 3   | E     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |

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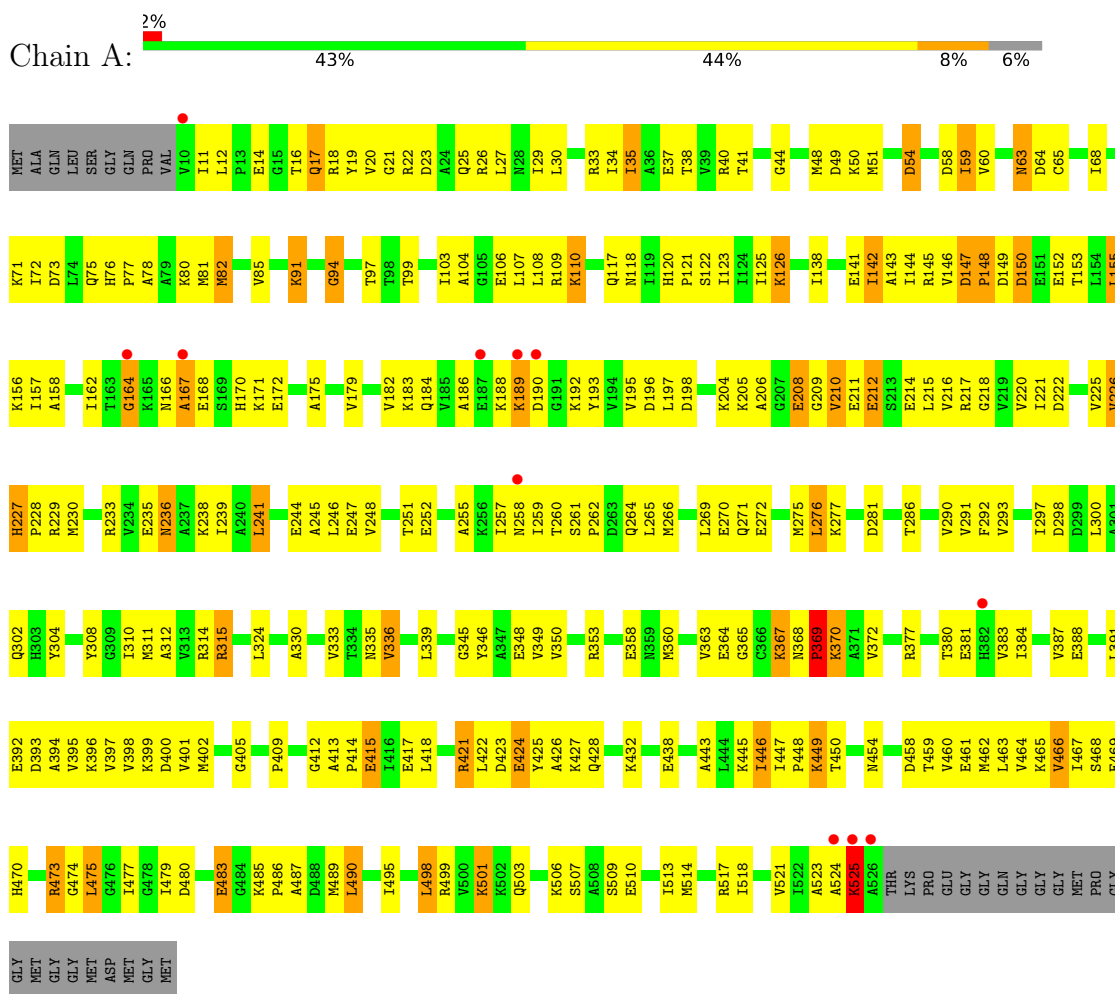
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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

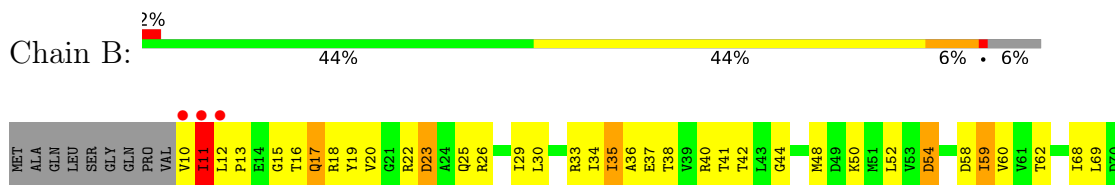
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Thermosome alpha subunit



#### • Molecule 1: Thermosome alpha subunit





Chain D: ■ 2% ■ 39% ■ 47% ■ 8% ■ 6%

|      |      |      |      |      |      |      |      |     |     |
|------|------|------|------|------|------|------|------|-----|-----|
| E510 | D443 | A442 | K370 | F292 | L221 | E152 | H76  | MET | VAL |
| I513 | A443 | A443 | K370 | Q294 | D222 | T153 | P77  | ALA | PRO |
| M514 | L444 | L444 | V372 | Q294 | V226 | L154 | A78  | GLN | VAL |
| I515 | K445 | K445 | V372 | Q294 | H227 | L155 | A79  | LEU | VAL |
| I516 | I446 | I446 | R377 | D298 | P298 | I157 | M81  | SER | VAL |
| R517 | I447 | I447 | R377 | D299 | R230 | A158 | M82  | GLY | VAL |
| P448 | P448 | P448 | T380 | L300 | R230 | I162 | Q89  | PRO | VAL |
| K449 | K449 | K449 | H382 | A301 | E235 | T163 | D90  | VAL | VAL |
| T450 | T450 | T450 | H382 | Q302 | E235 | G164 | E91  | V10 | VAL |
| L451 | L451 | L451 | V383 | H303 | A236 | K165 | E92  | I11 | VAL |
| A523 | A523 | A523 | I384 | V304 | K238 | N166 | A93  | I12 | VAL |
| A524 | A524 | A524 | V387 | L305 | K238 | A167 | G94  | P13 | VAL |
| K525 | V460 | E461 | E388 | Y308 | L241 | E168 | Q89  | E14 | VAL |
| A526 | M462 | E461 | E388 | G309 | I242 | I168 | D90  | G15 | VAL |
| THR  | L463 | L391 | L391 | I310 | N243 | S169 | E91  | T16 | VAL |
| PRO  | V464 | E392 | E392 | M311 | E244 | H170 | T98  | Q17 | VAL |
| GLU  | K465 | D393 | D393 | A312 | L245 | K171 | T99  | R18 | VAL |
| GLY  | V466 | A394 | A394 | V313 | E247 | E172 | A100 |     | VAL |
| GLY  | I467 | V395 | V395 | R314 | E247 | A175 | V101 | Q25 | VAL |
| GLN  | S468 | K396 | K396 | V248 | V248 | V179 | I103 | R26 | VAL |
| GLY  | E469 | V397 | V397 | V316 | K249 | E180 | G106 | I29 | VAL |
| GLY  | H470 | K398 | K398 | K317 | K250 | A191 | E106 | A31 | VAL |
| GLY  | G474 | D400 | D400 | R318 | T251 | N182 | L107 | A32 | VAL |
| MET  | L475 | V401 | V401 | S319 | E252 | K183 | L108 | R33 | VAL |
| PRO  | G476 | H401 | H401 | D320 | T253 | A186 | R109 | I34 | VAL |
| GLY  | I477 | D404 | D404 | M321 | D254 | E187 | K110 | I35 | VAL |
| GLY  | G478 | G405 | G405 | K323 | I257 | K188 | L114 | A36 | VAL |
| MET  | I479 | P409 | P409 | L324 | N258 | K189 | L115 | E37 | VAL |
| GLY  | D480 | A410 | A410 | A330 | T260 | D190 | D116 | T38 | VAL |
| MET  | E483 | G411 | G411 | K331 | S261 | G191 | Q117 | V39 | VAL |
| ASP  | G484 | G412 | G412 | L332 | Q264 | N193 | N118 | R40 | VAL |
| GLY  | K485 | A413 | A413 | V336 | L265 | V194 | I119 | G44 | VAL |
| GLY  | P414 | E415 | E415 | V336 | L266 | V195 | I123 | P45 | VAL |
| MET  | A486 | E416 | E416 | L339 | N266 | D196 | I124 | K50 | VAL |
| GLY  | D488 | E417 | E417 | E342 | F268 | L197 | I125 | M51 | VAL |
| MET  | M489 | L418 | L418 | E342 | L269 | D198 | K126 | D54 | VAL |
| ASP  | L490 | E421 | E421 | E348 | E270 | K201 | L130 | G57 | VAL |
| GLY  | E491 | L422 | L422 | V349 | Q271 | K204 | L134 | G57 | VAL |
| GLY  | K492 | D423 | D423 | V350 | E272 | K204 | K134 | D58 | VAL |
| GLY  | G493 | E424 | E424 | V350 | N275 | K205 | A135 | I59 | VAL |
| GLY  | I494 | E424 | E424 | V350 | L276 | A206 | Q136 | V60 | VAL |
| GLY  | I495 | E425 | E425 | R353 | L276 | G207 | E137 | V61 | VAL |
| GLY  | E496 | K426 | K426 | V354 |      |      |      |     |     |

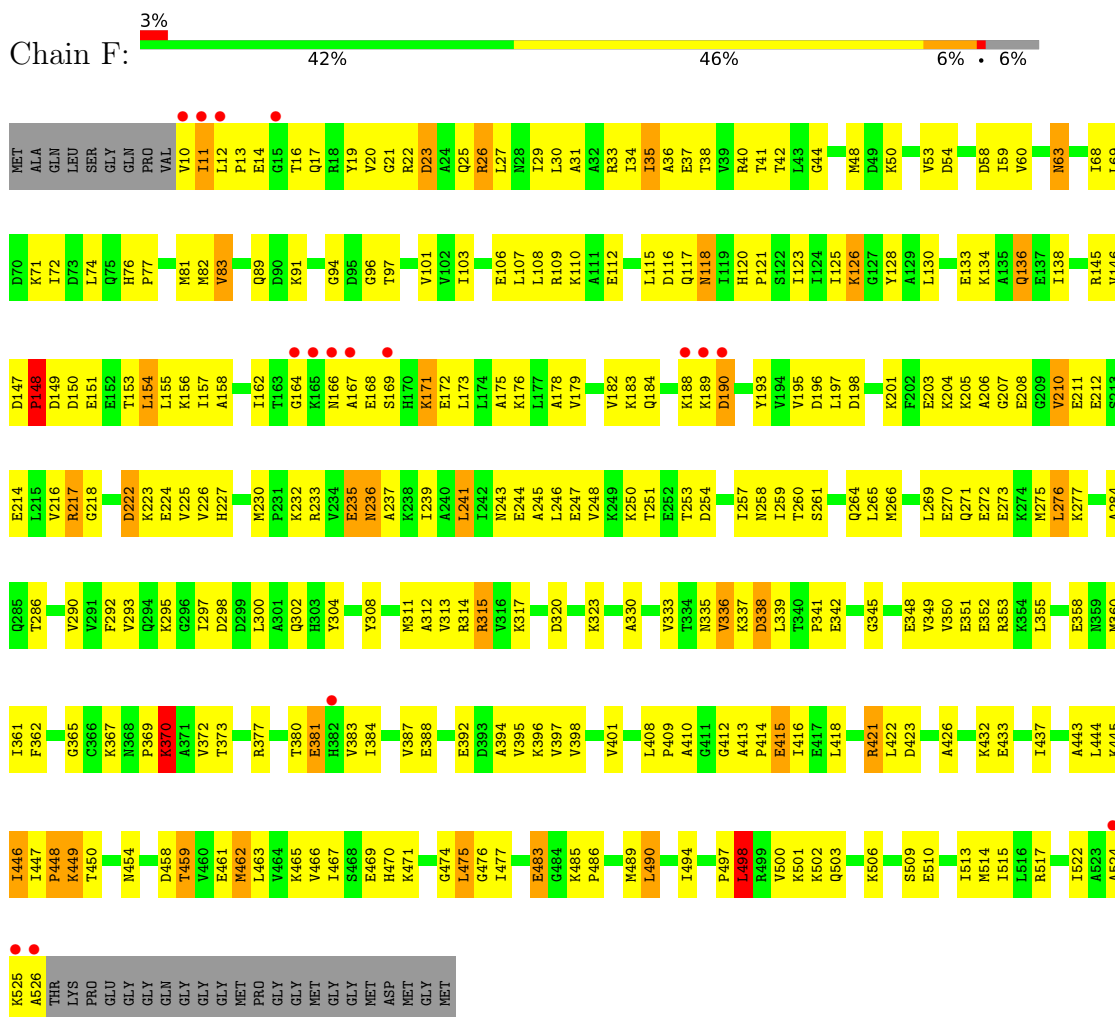
Chain E:

2% 38% 49% 7% 6%

MET ALA GLN LEU SER GLY GLN PRO VAL I11 I12 P13 E14 G15 T16 Q17 R18 Y19 V20 G21 R22 D23 R26 I29 L30 A31 A32 R33 I34 A36 E37 T38 V39 T41 T42 I43 G44 P45 G47 M48 D49 K50 M51 D54 D58 I59 V60 I68 L69 D70 D71 I72 D73 L74 Q75 H76 P77 K80 M81 M82 V83 E84 V85 K91 E92 A93 G94 T99 A100 V101 V102 I103 E106 L107 L108 R109 K110 L114 D116 Q117 N118 I119 H120 P121 T122 S122 I123 I124 I125 K126 L130 K134 A135 Q136 E137 I138 I142 A143 I144 R145 V146 D147 D148

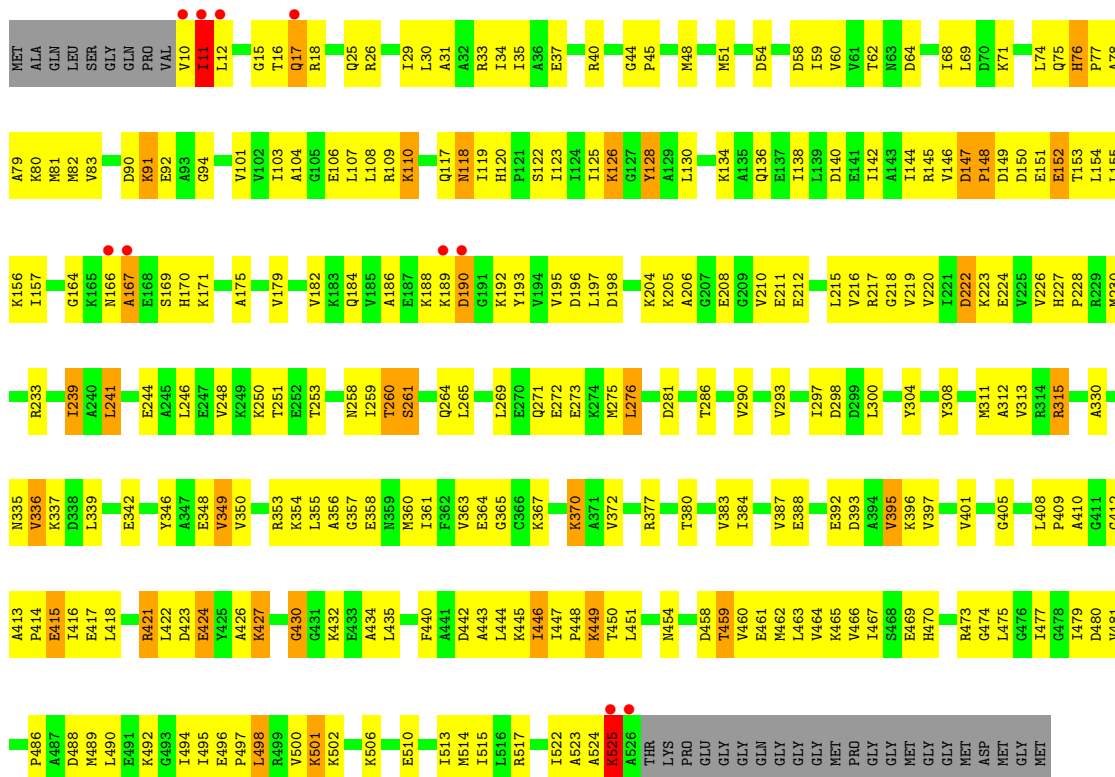


- Molecule 1: Thermosome alpha subunit

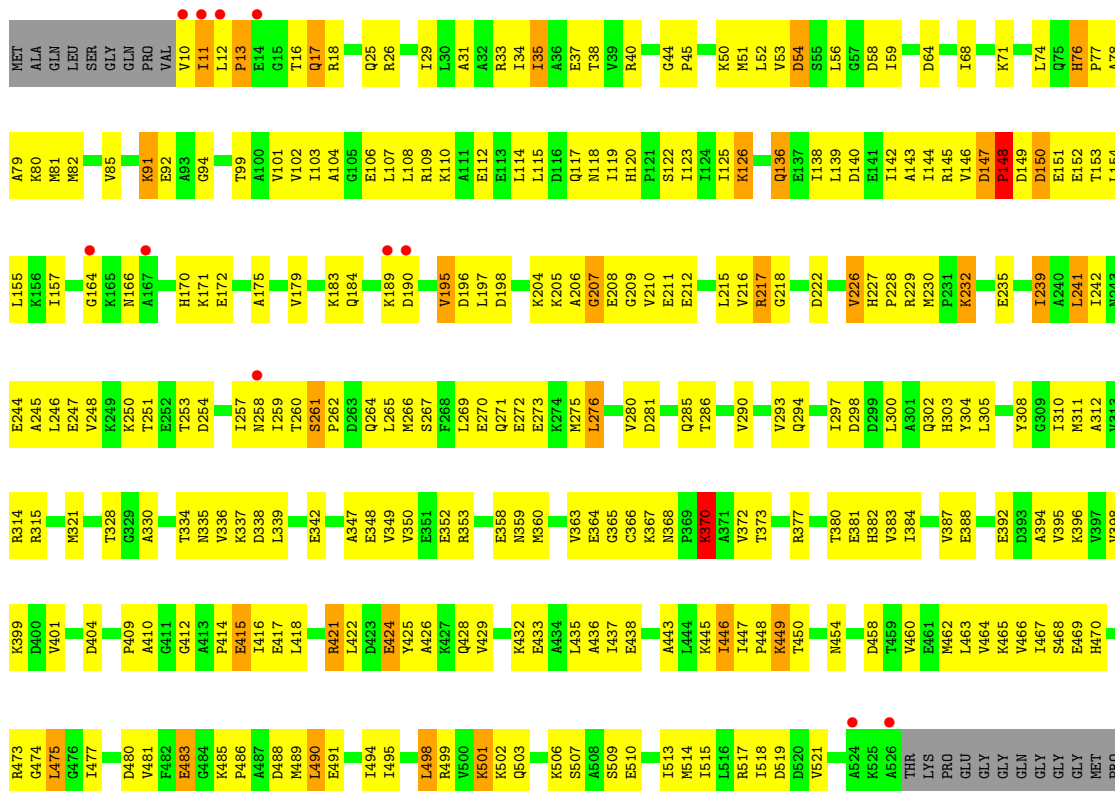


- Molecule 1: Thermosome alpha subunit





- Molecule 1: Thermosome alpha subunit



GLY  
GLY  
MET  
GLY  
GLY  
MET  
ASP  
MET  
GLY  
MET

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 207.43Å 236.23Å 234.11Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 73.62 – 3.00<br>73.62 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.0 (73.62-3.00)<br>98.1 (73.62-3.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.12                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.93 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.251 , 0.288<br>0.240 , 0.279                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5646 reflections (5.03%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 42.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.386                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 32.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                        | EDS              |
| Total number of atoms                                                   | 31751                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 38.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.59         | 2/3976 (0.1%)  | 1.03        | 19/5358 (0.4%)   |
| 1   | B     | 0.61         | 1/3976 (0.0%)  | 1.04        | 16/5358 (0.3%)   |
| 1   | C     | 0.58         | 2/3976 (0.1%)  | 1.04        | 21/5358 (0.4%)   |
| 1   | D     | 0.56         | 1/3976 (0.0%)  | 1.04        | 19/5358 (0.4%)   |
| 1   | E     | 0.56         | 1/3976 (0.0%)  | 1.03        | 13/5358 (0.2%)   |
| 1   | F     | 0.57         | 0/3976         | 1.02        | 14/5358 (0.3%)   |
| 1   | G     | 0.55         | 0/3976         | 1.00        | 16/5358 (0.3%)   |
| 1   | H     | 0.56         | 0/3976         | 1.01        | 18/5358 (0.3%)   |
| All | All   | 0.58         | 7/31808 (0.0%) | 1.02        | 136/42864 (0.3%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | C     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 11  | ILE  | CA-CB | 6.61  | 1.61        | 1.55     |
| 1   | C     | 514 | MET  | SD-CE | 6.24  | 1.95        | 1.79     |
| 1   | C     | 208 | GLU  | CA-C  | 5.78  | 1.61        | 1.53     |
| 1   | A     | 369 | PRO  | CA-C  | -5.61 | 1.45        | 1.52     |
| 1   | D     | 525 | LYS  | CA-C  | 5.51  | 1.59        | 1.53     |
| 1   | E     | 514 | MET  | SD-CE | 5.48  | 1.93        | 1.79     |
| 1   | A     | 192 | LYS  | N-CA  | 5.42  | 1.52        | 1.45     |

All (136) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 207 | GLY  | O-C-N      | -11.22 | 108.95      | 122.87   |
| 1   | C     | 117 | GLN  | OE1-CD-NE2 | -9.34  | 113.26      | 122.60   |
| 1   | F     | 474 | GLY  | N-CA-C     | 9.26   | 122.97      | 111.85   |
| 1   | B     | 44  | GLY  | CA-C-N     | 7.97   | 127.61      | 119.56   |
| 1   | B     | 44  | GLY  | C-N-CA     | 7.97   | 127.61      | 119.56   |
| 1   | C     | 44  | GLY  | CA-C-N     | 7.83   | 127.89      | 119.28   |
| 1   | C     | 44  | GLY  | C-N-CA     | 7.83   | 127.89      | 119.28   |
| 1   | F     | 83  | VAL  | N-CA-C     | -7.49  | 102.84      | 111.00   |
| 1   | D     | 238 | LYS  | N-CA-C     | -7.39  | 95.08       | 108.02   |
| 1   | E     | 239 | ILE  | N-CA-C     | 7.26   | 118.74      | 108.36   |
| 1   | H     | 44  | GLY  | CA-C-N     | 7.20   | 127.20      | 119.28   |
| 1   | H     | 44  | GLY  | C-N-CA     | 7.20   | 127.20      | 119.28   |
| 1   | G     | 226 | VAL  | N-CA-C     | 7.13   | 119.97      | 111.05   |
| 1   | B     | 474 | GLY  | N-CA-C     | 7.03   | 121.82      | 111.76   |
| 1   | F     | 44  | GLY  | CA-C-N     | 7.03   | 127.18      | 119.87   |
| 1   | F     | 44  | GLY  | C-N-CA     | 7.03   | 127.18      | 119.87   |
| 1   | D     | 44  | GLY  | CA-C-N     | 6.90   | 126.51      | 119.19   |
| 1   | D     | 44  | GLY  | C-N-CA     | 6.90   | 126.51      | 119.19   |
| 1   | E     | 44  | GLY  | CA-C-N     | 6.81   | 126.44      | 119.56   |
| 1   | E     | 44  | GLY  | C-N-CA     | 6.81   | 126.44      | 119.56   |
| 1   | A     | 239 | ILE  | N-CA-C     | 6.79   | 118.07      | 108.36   |
| 1   | C     | 474 | GLY  | N-CA-C     | 6.71   | 119.35      | 111.63   |
| 1   | D     | 227 | HIS  | CA-C-N     | 6.69   | 126.20      | 119.24   |
| 1   | D     | 227 | HIS  | C-N-CA     | 6.69   | 126.20      | 119.24   |
| 1   | H     | 147 | ASP  | CA-C-N     | 6.69   | 128.20      | 119.84   |
| 1   | H     | 147 | ASP  | C-N-CA     | 6.69   | 128.20      | 119.84   |
| 1   | A     | 474 | GLY  | N-CA-C     | 6.63   | 118.81      | 112.04   |
| 1   | F     | 63  | ASN  | N-CA-C     | -6.58  | 104.97      | 114.12   |
| 1   | H     | 239 | ILE  | N-CA-C     | 6.50   | 118.76      | 108.87   |
| 1   | D     | 207 | GLY  | N-CA-C     | -6.46  | 105.81      | 111.95   |
| 1   | B     | 15  | GLY  | N-CA-C     | -6.46  | 106.41      | 115.32   |
| 1   | A     | 208 | GLU  | CA-C-N     | -6.44  | 117.74      | 122.18   |
| 1   | A     | 208 | GLU  | C-N-CA     | -6.44  | 117.74      | 122.18   |
| 1   | C     | 117 | GLN  | CG-CD-NE2  | 6.44   | 126.06      | 116.40   |
| 1   | F     | 239 | ILE  | N-CA-C     | 6.38   | 117.48      | 108.36   |
| 1   | E     | 136 | GLN  | N-CA-C     | -6.38  | 104.25      | 111.07   |
| 1   | H     | 474 | GLY  | N-CA-C     | 6.38   | 118.96      | 111.63   |
| 1   | D     | 63  | ASN  | N-CA-C     | -6.37  | 105.15      | 114.39   |
| 1   | H     | 207 | GLY  | N-CA-C     | -6.34  | 105.92      | 111.95   |
| 1   | C     | 147 | ASP  | CA-C-N     | 6.33   | 127.76      | 119.84   |
| 1   | C     | 147 | ASP  | C-N-CA     | 6.33   | 127.76      | 119.84   |
| 1   | E     | 242 | ILE  | N-CA-C     | 6.33   | 117.24      | 107.99   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 474 | GLY  | N-CA-C | 6.31  | 118.88      | 111.63   |
| 1   | A     | 227 | HIS  | CA-C-N | 6.25  | 125.74      | 119.24   |
| 1   | A     | 227 | HIS  | C-N-CA | 6.25  | 125.74      | 119.24   |
| 1   | A     | 44  | GLY  | CA-C-N | 6.21  | 125.95      | 119.05   |
| 1   | A     | 44  | GLY  | C-N-CA | 6.21  | 125.95      | 119.05   |
| 1   | D     | 474 | GLY  | N-CA-C | 6.21  | 118.78      | 111.63   |
| 1   | D     | 525 | LYS  | N-CA-C | 6.18  | 118.09      | 107.28   |
| 1   | A     | 226 | VAL  | N-CA-C | 6.16  | 118.75      | 111.05   |
| 1   | D     | 226 | VAL  | N-CA-C | 6.11  | 119.60      | 111.17   |
| 1   | H     | 368 | ASN  | N-CA-C | -6.09 | 98.22       | 108.94   |
| 1   | G     | 239 | ILE  | N-CA-C | 6.05  | 117.39      | 109.58   |
| 1   | G     | 62  | THR  | N-CA-C | 6.01  | 117.92      | 108.96   |
| 1   | D     | 460 | VAL  | N-CA-C | 6.01  | 116.48      | 110.23   |
| 1   | A     | 525 | LYS  | N-CA-C | 6.00  | 120.33      | 107.67   |
| 1   | B     | 207 | GLY  | N-CA-C | -5.98 | 105.59      | 112.29   |
| 1   | H     | 195 | VAL  | N-CA-C | 5.95  | 116.43      | 107.80   |
| 1   | B     | 226 | VAL  | N-CA-C | 5.95  | 120.45      | 111.89   |
| 1   | H     | 226 | VAL  | N-CA-C | 5.94  | 120.44      | 111.89   |
| 1   | B     | 525 | LYS  | N-CA-C | 5.94  | 120.08      | 107.67   |
| 1   | G     | 525 | LYS  | N-CA-C | 5.90  | 117.61      | 107.28   |
| 1   | D     | 524 | ALA  | N-CA-C | 5.89  | 120.59      | 113.41   |
| 1   | F     | 261 | SER  | CA-C-N | 5.88  | 126.02      | 119.32   |
| 1   | F     | 261 | SER  | C-N-CA | 5.88  | 126.02      | 119.32   |
| 1   | A     | 238 | LYS  | N-CA-C | -5.83 | 98.23       | 108.20   |
| 1   | B     | 62  | THR  | N-CA-C | 5.81  | 117.90      | 109.07   |
| 1   | A     | 164 | GLY  | N-CA-C | -5.78 | 99.48       | 113.18   |
| 1   | A     | 167 | ALA  | N-CA-C | 5.77  | 123.09      | 110.80   |
| 1   | B     | 264 | GLN  | N-CA-C | 5.73  | 118.30      | 111.71   |
| 1   | G     | 223 | LYS  | N-CA-C | -5.73 | 100.42      | 108.96   |
| 1   | C     | 261 | SER  | CA-C-N | 5.69  | 126.96      | 119.84   |
| 1   | C     | 261 | SER  | C-N-CA | 5.69  | 126.96      | 119.84   |
| 1   | E     | 474 | GLY  | N-CA-C | 5.69  | 121.71      | 112.61   |
| 1   | F     | 498 | LEU  | N-CA-C | -5.68 | 105.85      | 112.89   |
| 1   | A     | 63  | ASN  | N-CA-C | -5.67 | 106.36      | 113.72   |
| 1   | E     | 291 | VAL  | N-CA-C | 5.64  | 116.01      | 108.11   |
| 1   | F     | 210 | VAL  | N-CA-C | -5.63 | 105.68      | 113.00   |
| 1   | G     | 261 | SER  | CA-C-N | 5.61  | 126.85      | 119.84   |
| 1   | G     | 261 | SER  | C-N-CA | 5.61  | 126.85      | 119.84   |
| 1   | H     | 261 | SER  | CA-C-N | 5.55  | 126.78      | 119.84   |
| 1   | H     | 261 | SER  | C-N-CA | 5.55  | 126.78      | 119.84   |
| 1   | E     | 525 | LYS  | N-CA-C | 5.51  | 117.68      | 107.60   |
| 1   | A     | 225 | VAL  | N-CA-C | -5.49 | 101.59      | 108.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | H     | 76  | HIS  | CA-C-N  | 5.47  | 124.66      | 118.97   |
| 1   | H     | 76  | HIS  | C-N-CA  | 5.47  | 124.66      | 118.97   |
| 1   | A     | 147 | ASP  | CA-C-N  | 5.46  | 126.67      | 119.84   |
| 1   | A     | 147 | ASP  | C-N-CA  | 5.46  | 126.67      | 119.84   |
| 1   | C     | 63  | ASN  | N-CA-C  | -5.44 | 107.01      | 113.97   |
| 1   | F     | 448 | PRO  | N-CA-C  | -5.43 | 105.98      | 113.53   |
| 1   | C     | 424 | GLU  | N-CA-C  | -5.40 | 105.29      | 111.07   |
| 1   | A     | 523 | ALA  | N-CA-C  | 5.39  | 118.34      | 109.72   |
| 1   | D     | 147 | ASP  | CA-C-N  | 5.38  | 126.56      | 119.84   |
| 1   | D     | 147 | ASP  | C-N-CA  | 5.38  | 126.56      | 119.84   |
| 1   | E     | 238 | LYS  | N-CA-C  | -5.37 | 98.48       | 107.99   |
| 1   | E     | 495 | ILE  | N-CA-C  | 5.37  | 116.44      | 108.65   |
| 1   | G     | 76  | HIS  | CA-C-N  | 5.37  | 124.83      | 119.24   |
| 1   | G     | 76  | HIS  | C-N-CA  | 5.37  | 124.83      | 119.24   |
| 1   | D     | 14  | GLU  | N-CA-C  | -5.34 | 103.48      | 110.53   |
| 1   | C     | 194 | VAL  | N-CA-C  | -5.34 | 100.96      | 108.27   |
| 1   | F     | 370 | LYS  | N-CA-C  | -5.33 | 106.00      | 112.88   |
| 1   | G     | 147 | ASP  | CA-C-N  | 5.33  | 126.50      | 119.84   |
| 1   | G     | 147 | ASP  | C-N-CA  | 5.33  | 126.50      | 119.84   |
| 1   | G     | 451 | LEU  | N-CA-C  | -5.30 | 105.08      | 112.45   |
| 1   | A     | 82  | MET  | N-CA-C  | -5.30 | 105.95      | 112.90   |
| 1   | B     | 261 | SER  | CA-C-N  | 5.30  | 126.47      | 119.84   |
| 1   | B     | 261 | SER  | C-N-CA  | 5.30  | 126.47      | 119.84   |
| 1   | H     | 370 | LYS  | N-CA-C  | -5.29 | 106.50      | 113.17   |
| 1   | E     | 475 | LEU  | N-CA-C  | 5.29  | 122.06      | 110.80   |
| 1   | F     | 136 | GLN  | N-CA-C  | -5.28 | 105.43      | 111.14   |
| 1   | H     | 424 | GLU  | N-CA-C  | -5.26 | 105.22      | 111.69   |
| 1   | B     | 148 | PRO  | CB-CA-C | 5.25  | 120.23      | 111.56   |
| 1   | C     | 208 | GLU  | CB-CA-C | -5.25 | 108.96      | 115.89   |
| 1   | C     | 370 | LYS  | N-CA-C  | -5.25 | 106.56      | 113.17   |
| 1   | D     | 237 | ALA  | N-CA-C  | 5.25  | 118.05      | 110.28   |
| 1   | C     | 62  | THR  | N-CA-C  | 5.25  | 116.95      | 109.14   |
| 1   | C     | 227 | HIS  | CA-C-N  | 5.24  | 125.30      | 119.32   |
| 1   | C     | 227 | HIS  | C-N-CA  | 5.24  | 125.30      | 119.32   |
| 1   | B     | 225 | VAL  | N-CA-C  | -5.22 | 102.00      | 108.89   |
| 1   | B     | 523 | ALA  | N-CA-C  | 5.22  | 118.07      | 109.72   |
| 1   | H     | 136 | GLN  | N-CA-C  | -5.20 | 104.86      | 111.11   |
| 1   | E     | 15  | GLY  | N-CA-C  | -5.20 | 108.44      | 115.36   |
| 1   | G     | 424 | GLU  | N-CA-C  | -5.17 | 105.53      | 111.07   |
| 1   | G     | 44  | GLY  | CA-C-N  | 5.16  | 124.78      | 119.05   |
| 1   | G     | 44  | GLY  | C-N-CA  | 5.16  | 124.78      | 119.05   |
| 1   | D     | 448 | PRO  | N-CA-C  | -5.15 | 106.08      | 113.75   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 59  | ILE  | N-CA-C | 5.14  | 115.37      | 108.17   |
| 1   | F     | 214 | GLU  | N-CA-C | 5.12  | 116.08      | 108.60   |
| 1   | D     | 242 | ILE  | N-CA-C | 5.12  | 114.94      | 107.37   |
| 1   | C     | 116 | ASP  | N-CA-C | -5.07 | 105.64      | 111.07   |
| 1   | H     | 232 | LYS  | N-CA-C | -5.06 | 106.95      | 113.02   |
| 1   | B     | 164 | GLY  | N-CA-C | -5.05 | 101.20      | 113.18   |
| 1   | B     | 448 | PRO  | N-CA-C | -5.05 | 106.63      | 113.40   |
| 1   | D     | 171 | LYS  | N-CA-C | -5.04 | 105.91      | 111.71   |
| 1   | E     | 237 | ALA  | N-CA-C | 5.01  | 117.48      | 109.96   |
| 1   | C     | 475 | LEU  | N-CA-C | 5.01  | 118.16      | 111.75   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 207 | GLY  | Mainchain |
| 1   | E     | 207 | GLY  | Mainchain |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3941  | 0        | 4122     | 287     | 0            |
| 1   | B     | 3941  | 0        | 4122     | 268     | 0            |
| 1   | C     | 3941  | 0        | 4122     | 283     | 0            |
| 1   | D     | 3941  | 0        | 4122     | 309     | 0            |
| 1   | E     | 3941  | 0        | 4122     | 345     | 0            |
| 1   | F     | 3941  | 0        | 4122     | 286     | 0            |
| 1   | G     | 3941  | 0        | 4122     | 266     | 0            |
| 1   | H     | 3941  | 0        | 4122     | 285     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | A     | 27    | 0        | 12       | 0       | 0            |
| 3   | B     | 27    | 0        | 12       | 1       | 0            |
| 3   | C     | 27    | 0        | 12       | 0       | 0            |
| 3   | D     | 27    | 0        | 12       | 0       | 0            |
| 3   | E     | 27    | 0        | 12       | 0       | 0            |
| 3   | F     | 27    | 0        | 12       | 1       | 0            |
| 3   | G     | 27    | 0        | 12       | 2       | 0            |
| 3   | H     | 27    | 0        | 12       | 1       | 0            |
| All | All   | 31751 | 0        | 33072    | 2202    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (2202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:380:THR:HG22 | 1:D:383:VAL:HG23 | 1.26                     | 1.15              |
| 1:H:380:THR:HG22 | 1:H:383:VAL:HG23 | 1.27                     | 1.14              |
| 1:E:380:THR:HG22 | 1:E:383:VAL:HG23 | 1.23                     | 1.11              |
| 1:A:380:THR:HG22 | 1:A:383:VAL:HG23 | 1.10                     | 1.09              |
| 1:B:380:THR:HG22 | 1:B:383:VAL:HG23 | 1.34                     | 1.09              |
| 1:C:10:VAL:HG22  | 1:C:11:ILE:H     | 1.19                     | 1.07              |
| 1:H:106:GLU:HG3  | 1:H:446:ILE:HG12 | 1.07                     | 1.06              |
| 1:B:10:VAL:HG22  | 1:B:11:ILE:H     | 1.20                     | 1.05              |
| 1:C:380:THR:HG22 | 1:C:383:VAL:HG23 | 1.39                     | 1.05              |
| 1:D:10:VAL:HG22  | 1:D:11:ILE:H     | 1.22                     | 1.03              |
| 1:E:10:VAL:HG22  | 1:E:11:ILE:H     | 1.19                     | 1.03              |
| 1:C:258:ASN:HB3  | 1:D:258:ASN:HD21 | 1.25                     | 1.02              |
| 1:H:261:SER:H    | 1:H:264:GLN:HE21 | 1.03                     | 1.00              |
| 1:A:166:ASN:HA   | 1:B:517:ARG:HH12 | 1.25                     | 1.00              |
| 1:C:60:VAL:HG21  | 1:C:71:LYS:HE2   | 1.42                     | 0.99              |
| 1:A:258:ASN:HD21 | 1:H:258:ASN:HB3  | 1.27                     | 0.99              |
| 1:G:380:THR:HG22 | 1:G:383:VAL:HG23 | 1.42                     | 0.99              |
| 1:C:260:THR:H    | 1:C:264:GLN:HE21 | 1.01                     | 0.98              |
| 1:G:421:ARG:HB2  | 1:G:421:ARG:HH11 | 1.24                     | 0.98              |
| 1:E:421:ARG:HH11 | 1:E:421:ARG:HB2  | 1.23                     | 0.98              |
| 1:E:12:LEU:HD23  | 1:E:13:PRO:HD2   | 1.47                     | 0.97              |
| 1:F:10:VAL:HG22  | 1:F:11:ILE:H     | 1.30                     | 0.96              |
| 1:H:260:THR:H    | 1:H:264:GLN:NE2  | 1.62                     | 0.96              |
| 1:B:260:THR:H    | 1:B:264:GLN:HE22 | 1.01                     | 0.94              |
| 1:E:125:ILE:HG23 | 1:E:513:ILE:HG23 | 1.46                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:421:ARG:HB2  | 1:F:421:ARG:HH11 | 1.29                     | 0.94              |
| 1:G:10:VAL:HG13  | 1:G:11:ILE:H     | 1.31                     | 0.94              |
| 1:D:258:ASN:HB3  | 1:E:258:ASN:HD21 | 1.30                     | 0.94              |
| 1:E:227:HIS:HB3  | 1:E:230:MET:HG3  | 1.50                     | 0.93              |
| 1:D:125:ILE:HG23 | 1:D:513:ILE:HG23 | 1.51                     | 0.93              |
| 1:A:260:THR:H    | 1:A:264:GLN:HE21 | 1.17                     | 0.92              |
| 1:D:260:THR:H    | 1:D:264:GLN:NE2  | 1.67                     | 0.92              |
| 1:H:106:GLU:HG3  | 1:H:446:ILE:CG1  | 1.98                     | 0.92              |
| 1:C:421:ARG:HB2  | 1:C:421:ARG:HH11 | 1.33                     | 0.91              |
| 1:F:380:THR:HG22 | 1:F:383:VAL:HG23 | 1.52                     | 0.91              |
| 1:F:125:ILE:HG23 | 1:F:513:ILE:HG23 | 1.50                     | 0.90              |
| 1:E:272:GLU:HA   | 1:E:275:MET:HE3  | 1.49                     | 0.90              |
| 1:E:230:MET:HE1  | 1:E:312:ALA:HB3  | 1.52                     | 0.89              |
| 1:A:230:MET:HE1  | 1:A:312:ALA:HB3  | 1.52                     | 0.89              |
| 1:B:260:THR:H    | 1:B:264:GLN:NE2  | 1.71                     | 0.89              |
| 1:A:166:ASN:HA   | 1:B:517:ARG:NH1  | 1.88                     | 0.89              |
| 1:E:260:THR:H    | 1:E:264:GLN:NE2  | 1.69                     | 0.89              |
| 1:H:125:ILE:HG23 | 1:H:513:ILE:HG23 | 1.52                     | 0.89              |
| 1:H:260:THR:H    | 1:H:264:GLN:HE22 | 1.19                     | 0.89              |
| 1:A:125:ILE:HG23 | 1:A:513:ILE:HG23 | 1.55                     | 0.88              |
| 1:H:106:GLU:CG   | 1:H:446:ILE:HG12 | 1.99                     | 0.88              |
| 1:D:383:VAL:O    | 1:D:387:VAL:HG23 | 1.74                     | 0.88              |
| 1:E:311:MET:HE1  | 1:E:350:VAL:HG12 | 1.54                     | 0.88              |
| 1:H:10:VAL:HG22  | 1:H:11:ILE:H     | 1.39                     | 0.88              |
| 1:H:380:THR:CG2  | 1:H:383:VAL:HG23 | 2.02                     | 0.88              |
| 1:G:258:ASN:HB3  | 1:H:258:ASN:HD21 | 1.36                     | 0.88              |
| 1:F:108:LEU:HD11 | 1:F:515:ILE:HD12 | 1.54                     | 0.87              |
| 1:B:184:GLN:NE2  | 1:B:217:ARG:HH21 | 1.72                     | 0.87              |
| 1:H:204:LYS:HB3  | 1:H:384:ILE:HG21 | 1.56                     | 0.87              |
| 1:A:212:GLU:HB2  | 1:A:377:ARG:HG3  | 1.56                     | 0.86              |
| 1:H:311:MET:HE1  | 1:H:350:VAL:HG12 | 1.57                     | 0.86              |
| 1:C:380:THR:CG2  | 1:C:383:VAL:HG23 | 2.03                     | 0.86              |
| 1:A:204:LYS:HD2  | 1:A:384:ILE:HG22 | 1.57                     | 0.86              |
| 1:E:293:VAL:HG21 | 1:E:297:ILE:HD11 | 1.56                     | 0.86              |
| 1:F:166:ASN:HA   | 1:G:517:ARG:HH12 | 1.41                     | 0.86              |
| 1:G:260:THR:H    | 1:G:264:GLN:HE21 | 1.21                     | 0.86              |
| 1:C:230:MET:HE1  | 1:C:312:ALA:HB3  | 1.58                     | 0.85              |
| 1:G:155:LEU:HD22 | 1:G:179:VAL:HG21 | 1.57                     | 0.85              |
| 1:G:54:ASP:OD1   | 1:G:58:ASP:HB3   | 1.76                     | 0.85              |
| 1:B:466:VAL:HG22 | 1:B:486:PRO:HG3  | 1.59                     | 0.85              |
| 1:D:421:ARG:HB2  | 1:D:421:ARG:HH11 | 1.42                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:81:MET:HE3   | 1:E:514:MET:SD   | 2.17                     | 0.84              |
| 1:F:524:ALA:O    | 1:F:525:LYS:HG3  | 1.77                     | 0.84              |
| 1:C:380:THR:HG23 | 1:C:383:VAL:H    | 1.40                     | 0.84              |
| 1:D:212:GLU:HB2  | 1:D:377:ARG:HG3  | 1.58                     | 0.84              |
| 1:E:72:ILE:HD11  | 1:F:522:ILE:HD12 | 1.56                     | 0.84              |
| 1:A:370:LYS:HE2  | 1:A:370:LYS:HA   | 1.60                     | 0.84              |
| 1:G:123:ILE:HG21 | 1:G:432:LYS:HB3  | 1.60                     | 0.84              |
| 1:G:260:THR:H    | 1:G:264:GLN:NE2  | 1.76                     | 0.84              |
| 1:A:204:LYS:HD3  | 1:A:388:GLU:OE2  | 1.76                     | 0.84              |
| 1:B:204:LYS:HB3  | 1:B:384:ILE:HG21 | 1.61                     | 0.83              |
| 1:C:409:PRO:HB3  | 1:C:490:LEU:CD1  | 2.07                     | 0.83              |
| 1:D:269:LEU:HD12 | 1:E:251:THR:HG23 | 1.58                     | 0.83              |
| 1:A:81:MET:HE3   | 1:A:514:MET:SD   | 2.19                     | 0.83              |
| 1:C:260:THR:H    | 1:C:264:GLN:NE2  | 1.76                     | 0.83              |
| 1:B:145:ARG:HG2  | 1:B:145:ARG:HH11 | 1.43                     | 0.83              |
| 1:F:260:THR:H    | 1:F:264:GLN:NE2  | 1.76                     | 0.83              |
| 1:G:462:MET:HA   | 1:G:462:MET:HE3  | 1.60                     | 0.83              |
| 1:D:290:VAL:HG22 | 1:D:311:MET:HE2  | 1.62                     | 0.82              |
| 1:A:206:ALA:HA   | 1:A:384:ILE:HD11 | 1.62                     | 0.82              |
| 1:B:380:THR:HG23 | 1:B:383:VAL:H    | 1.43                     | 0.82              |
| 1:G:265:LEU:O    | 1:G:269:LEU:HD13 | 1.79                     | 0.82              |
| 1:G:206:ALA:HA   | 1:G:384:ILE:HD11 | 1.62                     | 0.82              |
| 1:E:380:THR:CG2  | 1:E:383:VAL:HG23 | 2.07                     | 0.82              |
| 1:F:370:LYS:HE2  | 1:F:370:LYS:HA   | 1.61                     | 0.82              |
| 1:F:388:GLU:O    | 1:F:392:GLU:HG3  | 1.80                     | 0.82              |
| 1:E:179:VAL:O    | 1:E:183:LYS:HG3  | 1.80                     | 0.82              |
| 1:F:410:ALA:HB3  | 1:F:494:ILE:HG22 | 1.61                     | 0.82              |
| 1:H:227:HIS:HB3  | 1:H:230:MET:HG3  | 1.62                     | 0.82              |
| 1:A:469:GLU:HB2  | 1:A:477:ILE:HG21 | 1.60                     | 0.81              |
| 1:A:11:ILE:HG13  | 1:H:34:ILE:HG21  | 1.62                     | 0.81              |
| 1:B:421:ARG:HH11 | 1:B:421:ARG:HB2  | 1.44                     | 0.81              |
| 1:F:233:ARG:HH12 | 1:F:349:VAL:CG1  | 1.93                     | 0.81              |
| 1:F:380:THR:HG23 | 1:F:383:VAL:H    | 1.45                     | 0.81              |
| 1:F:445:LYS:O    | 1:F:449:LYS:HB2  | 1.81                     | 0.81              |
| 1:H:54:ASP:HB3   | 1:H:58:ASP:HB3   | 1.59                     | 0.81              |
| 1:A:138:ILE:HD13 | 1:A:421:ARG:HG2  | 1.61                     | 0.81              |
| 1:E:184:GLN:HA   | 1:E:184:GLN:HE21 | 1.45                     | 0.81              |
| 1:A:462:MET:O    | 1:A:466:VAL:HG23 | 1.81                     | 0.81              |
| 1:C:266:MET:O    | 1:C:270:GLU:HG3  | 1.81                     | 0.81              |
| 1:E:204:LYS:HD3  | 1:E:388:GLU:OE2  | 1.81                     | 0.81              |
| 1:A:38:THR:O     | 1:A:50:LYS:HE3   | 1.80                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:184:GLN:NE2  | 1:F:217:ARG:HH21 | 1.79                     | 0.80              |
| 1:A:380:THR:CG2  | 1:A:383:VAL:HG23 | 2.03                     | 0.80              |
| 1:B:315:ARG:HG3  | 1:B:315:ARG:HH11 | 1.45                     | 0.80              |
| 1:F:269:LEU:HD12 | 1:G:251:THR:HG23 | 1.63                     | 0.80              |
| 1:G:421:ARG:HB2  | 1:G:421:ARG:NH1  | 1.96                     | 0.80              |
| 1:C:144:ILE:HD11 | 1:C:490:LEU:HD21 | 1.62                     | 0.80              |
| 1:B:311:MET:HE1  | 1:B:350:VAL:HG12 | 1.63                     | 0.80              |
| 1:C:17:GLN:NE2   | 1:C:17:GLN:H     | 1.80                     | 0.80              |
| 1:C:462:MET:HE1  | 1:C:486:PRO:HD3  | 1.64                     | 0.80              |
| 1:G:380:THR:HG23 | 1:G:383:VAL:H    | 1.47                     | 0.80              |
| 1:B:81:MET:HE3   | 1:B:514:MET:SD   | 2.22                     | 0.80              |
| 1:G:370:LYS:HE2  | 1:G:370:LYS:HA   | 1.64                     | 0.80              |
| 1:D:204:LYS:HD2  | 1:D:384:ILE:HG22 | 1.64                     | 0.79              |
| 1:D:230:MET:HE1  | 1:D:312:ALA:HB3  | 1.62                     | 0.79              |
| 1:A:144:ILE:HD11 | 1:A:490:LEU:HD21 | 1.65                     | 0.79              |
| 1:A:269:LEU:HD12 | 1:B:251:THR:HG23 | 1.65                     | 0.79              |
| 1:E:348:GLU:HB3  | 1:E:365:GLY:HA3  | 1.64                     | 0.79              |
| 1:A:388:GLU:O    | 1:A:392:GLU:HG3  | 1.83                     | 0.79              |
| 1:A:421:ARG:HB2  | 1:A:421:ARG:HH11 | 1.48                     | 0.79              |
| 1:B:409:PRO:HB3  | 1:B:490:LEU:CD1  | 2.13                     | 0.79              |
| 1:D:241:LEU:HD22 | 1:D:330:ALA:HB3  | 1.65                     | 0.79              |
| 1:C:54:ASP:OD1   | 1:C:58:ASP:HB3   | 1.83                     | 0.78              |
| 1:C:483:GLU:HG3  | 1:C:485:LYS:NZ   | 1.97                     | 0.78              |
| 1:G:125:ILE:HD13 | 1:G:517:ARG:HG2  | 1.65                     | 0.78              |
| 1:B:445:LYS:O    | 1:B:448:PRO:HD2  | 1.82                     | 0.78              |
| 1:G:60:VAL:HG21  | 1:G:71:LYS:HE2   | 1.65                     | 0.78              |
| 1:G:125:ILE:HG23 | 1:G:513:ILE:HG23 | 1.66                     | 0.78              |
| 1:G:272:GLU:HA   | 1:G:275:MET:HE3  | 1.66                     | 0.78              |
| 1:H:370:LYS:HA   | 1:H:370:LYS:HE2  | 1.66                     | 0.78              |
| 1:A:380:THR:HG22 | 1:A:383:VAL:CG2  | 2.05                     | 0.78              |
| 1:D:81:MET:HE3   | 1:D:514:MET:SD   | 2.24                     | 0.77              |
| 1:E:409:PRO:HA   | 1:E:495:ILE:HG22 | 1.65                     | 0.77              |
| 1:A:204:LYS:HB3  | 1:A:384:ILE:CG2  | 2.15                     | 0.77              |
| 1:F:217:ARG:HA   | 1:F:372:VAL:HG23 | 1.67                     | 0.77              |
| 1:H:204:LYS:HD3  | 1:H:388:GLU:OE2  | 1.83                     | 0.77              |
| 1:C:10:VAL:HG22  | 1:C:11:ILE:N     | 1.99                     | 0.77              |
| 1:B:370:LYS:HE2  | 1:B:370:LYS:HA   | 1.64                     | 0.77              |
| 1:D:73:ASP:HB3   | 1:E:13:PRO:HG2   | 1.66                     | 0.77              |
| 1:E:233:ARG:HH12 | 1:E:349:VAL:CG1  | 1.97                     | 0.77              |
| 1:G:75:GLN:HG2   | 1:H:13:PRO:HD3   | 1.67                     | 0.77              |
| 1:H:272:GLU:HA   | 1:H:275:MET:HE3  | 1.67                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:166:ASN:HA   | 1:D:517:ARG:HH12 | 1.50                     | 0.76              |
| 1:C:462:MET:O    | 1:C:466:VAL:HG23 | 1.84                     | 0.76              |
| 1:D:265:LEU:O    | 1:D:269:LEU:HD13 | 1.85                     | 0.76              |
| 1:B:166:ASN:HA   | 1:C:517:ARG:HH12 | 1.50                     | 0.76              |
| 1:C:348:GLU:O    | 1:C:349:VAL:HG23 | 1.85                     | 0.76              |
| 1:F:260:THR:H    | 1:F:264:GLN:HE21 | 1.33                     | 0.76              |
| 1:B:272:GLU:HA   | 1:B:275:MET:HE3  | 1.66                     | 0.76              |
| 1:B:380:THR:CG2  | 1:B:383:VAL:HG23 | 2.16                     | 0.76              |
| 1:C:206:ALA:HA   | 1:C:384:ILE:HD11 | 1.67                     | 0.76              |
| 1:F:106:GLU:HG2  | 1:F:446:ILE:HG13 | 1.67                     | 0.76              |
| 1:E:466:VAL:HG22 | 1:E:486:PRO:HG3  | 1.68                     | 0.76              |
| 1:D:12:LEU:HD21  | 1:D:16:THR:HG21  | 1.68                     | 0.76              |
| 1:D:462:MET:HE1  | 1:D:486:PRO:HD3  | 1.68                     | 0.76              |
| 1:F:462:MET:O    | 1:F:466:VAL:HG23 | 1.85                     | 0.76              |
| 1:H:215:LEU:HD11 | 1:H:372:VAL:HG21 | 1.66                     | 0.76              |
| 1:G:204:LYS:HB3  | 1:G:384:ILE:HG21 | 1.67                     | 0.76              |
| 1:G:208:GLU:HB3  | 1:G:212:GLU:HG3  | 1.68                     | 0.76              |
| 1:C:125:ILE:HG23 | 1:C:513:ILE:HG23 | 1.67                     | 0.76              |
| 1:D:204:LYS:HB3  | 1:D:384:ILE:HG21 | 1.65                     | 0.76              |
| 1:B:10:VAL:HG22  | 1:B:11:ILE:N     | 1.98                     | 0.75              |
| 1:B:206:ALA:HA   | 1:B:384:ILE:HD11 | 1.68                     | 0.75              |
| 1:D:91:LYS:HB2   | 1:D:91:LYS:NZ    | 2.01                     | 0.75              |
| 1:E:380:THR:HG23 | 1:E:383:VAL:H    | 1.50                     | 0.75              |
| 1:G:144:ILE:HD11 | 1:G:490:LEU:HD21 | 1.66                     | 0.75              |
| 1:C:175:ALA:O    | 1:C:179:VAL:HG23 | 1.87                     | 0.75              |
| 1:D:217:ARG:HB3  | 1:D:217:ARG:NH1  | 2.00                     | 0.75              |
| 1:G:25:GLN:O     | 1:G:29:ILE:HG13  | 1.85                     | 0.75              |
| 1:G:244:GLU:OE1  | 1:G:336:VAL:HG22 | 1.85                     | 0.75              |
| 1:H:204:LYS:HB3  | 1:H:384:ILE:CG2  | 2.16                     | 0.75              |
| 1:A:369:PRO:O    | 1:A:370:LYS:HE2  | 1.85                     | 0.75              |
| 1:B:462:MET:HE1  | 1:B:486:PRO:HD3  | 1.67                     | 0.75              |
| 1:B:380:THR:HG22 | 1:B:383:VAL:CG2  | 2.14                     | 0.75              |
| 1:D:73:ASP:O     | 1:E:13:PRO:HD3   | 1.86                     | 0.75              |
| 1:G:82:MET:HE3   | 1:G:101:VAL:HG13 | 1.69                     | 0.75              |
| 1:G:142:ILE:HB   | 1:G:475:LEU:HD22 | 1.69                     | 0.75              |
| 1:D:94:GLY:HA3   | 1:D:396:LYS:HD2  | 1.67                     | 0.75              |
| 1:E:462:MET:O    | 1:E:466:VAL:HG23 | 1.86                     | 0.75              |
| 1:C:204:LYS:HB3  | 1:C:384:ILE:HG21 | 1.68                     | 0.74              |
| 1:D:380:THR:CG2  | 1:D:383:VAL:HG23 | 2.12                     | 0.74              |
| 1:F:466:VAL:HG22 | 1:F:486:PRO:HG3  | 1.67                     | 0.74              |
| 1:H:462:MET:HE1  | 1:H:486:PRO:HD3  | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:82:MET:HE3   | 1:C:101:VAL:HG13 | 1.68                     | 0.74              |
| 1:D:10:VAL:HG22  | 1:D:11:ILE:N     | 2.02                     | 0.74              |
| 1:H:136:GLN:NE2  | 1:H:502:LYS:HE3  | 2.02                     | 0.74              |
| 1:B:410:ALA:HB3  | 1:B:494:ILE:HG22 | 1.68                     | 0.74              |
| 1:G:166:ASN:HA   | 1:H:517:ARG:HH12 | 1.52                     | 0.74              |
| 1:A:290:VAL:HG22 | 1:A:311:MET:HE2  | 1.70                     | 0.74              |
| 1:D:94:GLY:CA    | 1:D:396:LYS:HD2  | 2.18                     | 0.74              |
| 1:H:447:ILE:HB   | 1:H:448:PRO:HD3  | 1.68                     | 0.74              |
| 1:E:11:ILE:HD13  | 1:E:11:ILE:C     | 2.12                     | 0.74              |
| 1:E:233:ARG:HH12 | 1:E:349:VAL:HG11 | 1.52                     | 0.74              |
| 1:D:469:GLU:HB2  | 1:D:477:ILE:HG21 | 1.69                     | 0.74              |
| 1:E:125:ILE:HG23 | 1:E:513:ILE:CG2  | 2.18                     | 0.74              |
| 1:A:447:ILE:HB   | 1:A:448:PRO:HD3  | 1.70                     | 0.74              |
| 1:F:446:ILE:O    | 1:F:450:THR:HG23 | 1.87                     | 0.74              |
| 1:D:205:LYS:HD2  | 1:D:356:ALA:HB3  | 1.69                     | 0.73              |
| 1:E:175:ALA:O    | 1:E:179:VAL:HG23 | 1.88                     | 0.73              |
| 1:F:315:ARG:HH11 | 1:F:315:ARG:HG3  | 1.52                     | 0.73              |
| 1:H:353:ARG:NH2  | 1:H:364:GLU:OE2  | 2.21                     | 0.73              |
| 1:A:251:THR:HG23 | 1:H:269:LEU:HD12 | 1.70                     | 0.73              |
| 1:G:138:ILE:HD13 | 1:G:421:ARG:HG2  | 1.70                     | 0.73              |
| 1:H:261:SER:H    | 1:H:264:GLN:NE2  | 1.83                     | 0.73              |
| 1:H:469:GLU:HB2  | 1:H:477:ILE:HG21 | 1.71                     | 0.73              |
| 1:A:258:ASN:HB3  | 1:B:258:ASN:HD21 | 1.52                     | 0.73              |
| 1:D:445:LYS:O    | 1:D:449:LYS:HB2  | 1.87                     | 0.73              |
| 1:G:466:VAL:HG22 | 1:G:486:PRO:HG3  | 1.69                     | 0.73              |
| 1:H:144:ILE:HD11 | 1:H:490:LEU:HD21 | 1.70                     | 0.73              |
| 1:A:462:MET:HE1  | 1:A:486:PRO:HD3  | 1.68                     | 0.73              |
| 1:C:447:ILE:HB   | 1:C:448:PRO:HD3  | 1.69                     | 0.73              |
| 1:H:206:ALA:HA   | 1:H:384:ILE:HD11 | 1.69                     | 0.73              |
| 1:E:204:LYS:HB3  | 1:E:384:ILE:HG21 | 1.68                     | 0.73              |
| 1:H:421:ARG:HH11 | 1:H:421:ARG:HB2  | 1.53                     | 0.73              |
| 1:A:155:LEU:HD22 | 1:A:179:VAL:HG21 | 1.71                     | 0.73              |
| 1:B:460:VAL:O    | 1:B:464:VAL:HG23 | 1.87                     | 0.73              |
| 1:A:204:LYS:HB3  | 1:A:384:ILE:HG21 | 1.69                     | 0.73              |
| 1:D:276:LEU:HD23 | 1:D:300:LEU:HB2  | 1.69                     | 0.73              |
| 1:B:488:ASP:HB3  | 1:B:491:GLU:HG3  | 1.71                     | 0.72              |
| 1:F:506:LYS:O    | 1:F:510:GLU:HG3  | 1.89                     | 0.72              |
| 1:H:230:MET:HE1  | 1:H:312:ALA:HB3  | 1.71                     | 0.72              |
| 1:F:82:MET:HE3   | 1:F:101:VAL:HG13 | 1.69                     | 0.72              |
| 1:H:443:ALA:O    | 1:H:446:ILE:HG13 | 1.89                     | 0.72              |
| 1:G:413:ALA:HB3  | 1:G:414:PRO:HD3  | 1.71                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:315:ARG:HH11 | 1:C:315:ARG:HG3  | 1.54                     | 0.72              |
| 1:H:462:MET:O    | 1:H:466:VAL:HG23 | 1.88                     | 0.72              |
| 1:A:75:GLN:HB2   | 1:B:11:ILE:C     | 2.14                     | 0.72              |
| 1:B:204:LYS:HD3  | 1:B:388:GLU:OE2  | 1.89                     | 0.72              |
| 1:C:311:MET:HE1  | 1:C:350:VAL:HG12 | 1.70                     | 0.72              |
| 1:G:134:LYS:O    | 1:G:138:ILE:HG13 | 1.90                     | 0.72              |
| 1:E:146:VAL:HG22 | 1:E:147:ASP:H    | 1.55                     | 0.72              |
| 1:A:383:VAL:O    | 1:A:387:VAL:HG23 | 1.88                     | 0.72              |
| 1:E:103:ILE:O    | 1:E:107:LEU:HB2  | 1.89                     | 0.72              |
| 1:B:125:ILE:HG23 | 1:B:513:ILE:HG23 | 1.70                     | 0.72              |
| 1:B:506:LYS:O    | 1:B:510:GLU:HG3  | 1.89                     | 0.72              |
| 1:D:60:VAL:HG21  | 1:D:71:LYS:HE2   | 1.71                     | 0.72              |
| 1:D:125:ILE:HD13 | 1:D:517:ARG:HG2  | 1.69                     | 0.72              |
| 1:D:123:ILE:HG21 | 1:D:432:LYS:HB2  | 1.71                     | 0.72              |
| 1:E:258:ASN:HB3  | 1:F:258:ASN:HD21 | 1.54                     | 0.72              |
| 1:G:59:ILE:HD12  | 1:G:59:ILE:N     | 2.05                     | 0.72              |
| 1:H:483:GLU:HG3  | 1:H:485:LYS:NZ   | 2.05                     | 0.72              |
| 1:D:315:ARG:HH11 | 1:D:315:ARG:HG3  | 1.52                     | 0.71              |
| 1:H:513:ILE:O    | 1:H:517:ARG:HG3  | 1.90                     | 0.71              |
| 1:G:473:ARG:HB2  | 1:G:477:ILE:HG13 | 1.72                     | 0.71              |
| 1:H:143:ALA:HB3  | 1:H:145:ARG:HH12 | 1.55                     | 0.71              |
| 1:H:266:MET:O    | 1:H:270:GLU:HG3  | 1.90                     | 0.71              |
| 1:E:311:MET:HE1  | 1:E:350:VAL:CG1  | 2.20                     | 0.71              |
| 1:A:82:MET:HE1   | 1:A:104:ALA:HB3  | 1.71                     | 0.71              |
| 1:F:54:ASP:OD1   | 1:F:58:ASP:HB3   | 1.90                     | 0.71              |
| 1:D:37:GLU:HG2   | 1:D:40:ARG:NH1   | 2.05                     | 0.71              |
| 1:A:22:ARG:HG3   | 1:A:23:ASP:N     | 2.06                     | 0.71              |
| 1:C:506:LYS:O    | 1:C:510:GLU:HG3  | 1.91                     | 0.71              |
| 1:E:147:ASP:HB3  | 1:E:150:ASP:HB2  | 1.71                     | 0.71              |
| 1:G:108:LEU:HD11 | 1:G:515:ILE:HD12 | 1.71                     | 0.71              |
| 1:B:286:THR:HG21 | 1:B:339:LEU:HG   | 1.72                     | 0.71              |
| 1:D:380:THR:HG22 | 1:D:383:VAL:CG2  | 2.14                     | 0.71              |
| 1:E:184:GLN:HA   | 1:E:184:GLN:NE2  | 2.06                     | 0.71              |
| 1:F:230:MET:HE1  | 1:F:312:ALA:HB3  | 1.73                     | 0.71              |
| 1:C:311:MET:HE1  | 1:C:350:VAL:CG1  | 2.21                     | 0.71              |
| 1:D:123:ILE:HG21 | 1:D:432:LYS:CB   | 2.21                     | 0.71              |
| 1:E:230:MET:HE1  | 1:E:312:ALA:CB   | 2.21                     | 0.71              |
| 1:F:11:ILE:O     | 1:F:11:ILE:HD13  | 1.90                     | 0.71              |
| 1:C:380:THR:HG22 | 1:C:383:VAL:CG2  | 2.19                     | 0.70              |
| 1:F:412:GLY:O    | 1:F:415:GLU:HG2  | 1.90                     | 0.70              |
| 1:D:311:MET:HE1  | 1:D:350:VAL:HG12 | 1.72                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:29:ILE:O     | 1:F:33:ARG:HG3   | 1.91                     | 0.70              |
| 1:C:383:VAL:O    | 1:C:387:VAL:HG23 | 1.91                     | 0.70              |
| 1:F:178:ALA:O    | 1:F:182:VAL:HG23 | 1.92                     | 0.70              |
| 1:F:147:ASP:HB3  | 1:F:150:ASP:HB2  | 1.73                     | 0.70              |
| 1:G:383:VAL:O    | 1:G:387:VAL:HG23 | 1.92                     | 0.70              |
| 1:H:445:LYS:O    | 1:H:449:LYS:HB2  | 1.92                     | 0.70              |
| 1:B:73:ASP:HB3   | 1:C:13:PRO:HG2   | 1.72                     | 0.70              |
| 1:B:392:GLU:O    | 1:B:396:LYS:HE3  | 1.92                     | 0.70              |
| 1:F:48:MET:HE2   | 1:F:48:MET:HA    | 1.74                     | 0.70              |
| 1:H:506:LYS:O    | 1:H:510:GLU:HG3  | 1.91                     | 0.70              |
| 1:C:25:GLN:O     | 1:C:29:ILE:HG13  | 1.92                     | 0.70              |
| 1:C:125:ILE:HD13 | 1:C:517:ARG:HG2  | 1.73                     | 0.70              |
| 1:C:466:VAL:HG22 | 1:C:486:PRO:HG3  | 1.71                     | 0.70              |
| 1:H:380:THR:HG22 | 1:H:383:VAL:CG2  | 2.16                     | 0.70              |
| 1:A:91:LYS:HB2   | 1:A:91:LYS:NZ    | 2.06                     | 0.70              |
| 1:B:446:ILE:O    | 1:B:450:THR:HG23 | 1.92                     | 0.70              |
| 1:E:483:GLU:HG3  | 1:E:485:LYS:NZ   | 2.06                     | 0.70              |
| 1:F:10:VAL:HG22  | 1:F:11:ILE:N     | 2.06                     | 0.70              |
| 1:F:509:SER:O    | 1:F:513:ILE:HG13 | 1.92                     | 0.70              |
| 1:G:460:VAL:O    | 1:G:464:VAL:HG23 | 1.91                     | 0.70              |
| 1:D:348:GLU:HB3  | 1:D:365:GLY:HA3  | 1.74                     | 0.70              |
| 1:B:462:MET:HA   | 1:B:462:MET:HE3  | 1.73                     | 0.70              |
| 1:H:261:SER:N    | 1:H:264:GLN:HE21 | 1.85                     | 0.70              |
| 1:A:244:GLU:OE1  | 1:A:336:VAL:HG22 | 1.91                     | 0.69              |
| 1:B:205:LYS:O    | 1:B:377:ARG:NH1  | 2.25                     | 0.69              |
| 1:F:233:ARG:HH12 | 1:F:349:VAL:HG11 | 1.54                     | 0.69              |
| 1:G:447:ILE:HB   | 1:G:448:PRO:HD3  | 1.74                     | 0.69              |
| 1:H:241:LEU:HD22 | 1:H:330:ALA:HB3  | 1.73                     | 0.69              |
| 1:H:394:ALA:O    | 1:H:398:VAL:HG23 | 1.91                     | 0.69              |
| 1:A:394:ALA:O    | 1:A:398:VAL:HG23 | 1.92                     | 0.69              |
| 1:B:42:THR:HG22  | 1:B:48:MET:O     | 1.90                     | 0.69              |
| 1:B:244:GLU:OE1  | 1:B:336:VAL:HG22 | 1.91                     | 0.69              |
| 1:C:412:GLY:O    | 1:C:415:GLU:HG2  | 1.91                     | 0.69              |
| 1:C:488:ASP:O    | 1:C:492:LYS:HG2  | 1.92                     | 0.69              |
| 1:D:37:GLU:HG2   | 1:D:40:ARG:HH12  | 1.58                     | 0.69              |
| 1:H:501:LYS:HA   | 1:H:501:LYS:HE3  | 1.74                     | 0.69              |
| 1:E:257:ILE:HG22 | 1:E:259:ILE:HD12 | 1.74                     | 0.69              |
| 1:E:276:LEU:HD23 | 1:E:300:LEU:HB2  | 1.75                     | 0.69              |
| 1:E:410:ALA:HB3  | 1:E:494:ILE:HG22 | 1.74                     | 0.69              |
| 1:G:311:MET:HE1  | 1:G:350:VAL:HG12 | 1.75                     | 0.69              |
| 1:A:48:MET:HE2   | 1:A:48:MET:HA    | 1.72                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:204:LYS:HB3  | 1:D:384:ILE:CG2  | 2.21                     | 0.69              |
| 1:F:380:THR:CG2  | 1:F:383:VAL:HG23 | 2.20                     | 0.69              |
| 1:B:30:LEU:O     | 1:B:34:ILE:HG13  | 1.93                     | 0.69              |
| 1:D:460:VAL:O    | 1:D:464:VAL:HG23 | 1.92                     | 0.69              |
| 1:F:227:HIS:HB3  | 1:F:230:MET:HG3  | 1.74                     | 0.69              |
| 1:G:409:PRO:HB3  | 1:G:490:LEU:CD1  | 2.22                     | 0.69              |
| 1:E:205:LYS:HZ1  | 1:E:358:GLU:HG2  | 1.57                     | 0.69              |
| 1:G:17:GLN:NE2   | 1:G:17:GLN:H     | 1.91                     | 0.69              |
| 1:E:12:LEU:HD23  | 1:E:13:PRO:CD    | 2.22                     | 0.69              |
| 1:E:421:ARG:HB2  | 1:E:421:ARG:NH1  | 2.05                     | 0.69              |
| 1:E:466:VAL:HG21 | 1:E:479:ILE:HG12 | 1.75                     | 0.69              |
| 1:F:409:PRO:HB3  | 1:F:490:LEU:HD13 | 1.73                     | 0.69              |
| 1:G:498:LEU:O    | 1:G:498:LEU:HD22 | 1.93                     | 0.69              |
| 1:H:123:ILE:HG21 | 1:H:432:LYS:HB3  | 1.74                     | 0.69              |
| 1:H:483:GLU:HG3  | 1:H:485:LYS:HZ3  | 1.58                     | 0.69              |
| 1:C:410:ALA:HB3  | 1:C:494:ILE:HG22 | 1.73                     | 0.69              |
| 1:E:269:LEU:HD12 | 1:F:251:THR:HG23 | 1.74                     | 0.69              |
| 1:A:196:ASP:OD1  | 1:A:198:ASP:HB2  | 1.92                     | 0.69              |
| 1:B:204:LYS:HB3  | 1:B:384:ILE:CG2  | 2.22                     | 0.69              |
| 1:H:226:VAL:HG12 | 1:H:312:ALA:O    | 1.93                     | 0.69              |
| 1:C:189:LYS:HD2  | 1:C:189:LYS:C    | 2.18                     | 0.68              |
| 1:G:29:ILE:HG23  | 1:G:108:LEU:HB3  | 1.74                     | 0.68              |
| 1:E:166:ASN:HA   | 1:F:517:ARG:NH1  | 2.09                     | 0.68              |
| 1:F:103:ILE:O    | 1:F:107:LEU:HB2  | 1.92                     | 0.68              |
| 1:A:258:ASN:ND2  | 1:H:258:ASN:HB3  | 2.05                     | 0.68              |
| 1:B:144:ILE:HD11 | 1:B:490:LEU:HD21 | 1.76                     | 0.68              |
| 1:G:230:MET:HE1  | 1:G:312:ALA:HB3  | 1.74                     | 0.68              |
| 1:H:304:TYR:O    | 1:H:308:TYR:HD1  | 1.76                     | 0.68              |
| 1:C:370:LYS:HE2  | 1:C:370:LYS:HA   | 1.74                     | 0.68              |
| 1:D:261:SER:O    | 1:D:264:GLN:HG3  | 1.92                     | 0.68              |
| 1:G:412:GLY:O    | 1:G:415:GLU:HG2  | 1.93                     | 0.68              |
| 1:A:175:ALA:O    | 1:A:179:VAL:HG23 | 1.93                     | 0.68              |
| 1:A:462:MET:HE3  | 1:A:462:MET:HA   | 1.74                     | 0.68              |
| 1:C:421:ARG:HB2  | 1:C:421:ARG:NH1  | 2.09                     | 0.68              |
| 1:G:144:ILE:CD1  | 1:G:490:LEU:HD21 | 2.23                     | 0.68              |
| 1:C:75:GLN:HG3   | 1:D:10:VAL:HG13  | 1.76                     | 0.68              |
| 1:C:445:LYS:O    | 1:C:448:PRO:HD2  | 1.93                     | 0.68              |
| 1:G:380:THR:CG2  | 1:G:383:VAL:HG23 | 2.23                     | 0.68              |
| 1:B:11:ILE:C     | 1:B:11:ILE:HD13  | 2.19                     | 0.68              |
| 1:D:506:LYS:O    | 1:D:510:GLU:HG3  | 1.94                     | 0.68              |
| 1:E:416:ILE:O    | 1:E:420:ILE:HG13 | 1.94                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:11:ILE:HD13  | 1:H:11:ILE:C     | 2.18                     | 0.68              |
| 1:A:260:THR:H    | 1:A:264:GLN:NE2  | 1.90                     | 0.68              |
| 1:D:217:ARG:HA   | 1:D:372:VAL:HG23 | 1.76                     | 0.68              |
| 1:D:443:ALA:O    | 1:D:446:ILE:HG13 | 1.93                     | 0.68              |
| 1:E:48:MET:HE2   | 1:E:48:MET:HA    | 1.76                     | 0.68              |
| 1:A:353:ARG:NH2  | 1:A:364:GLU:OE2  | 2.26                     | 0.68              |
| 1:C:446:ILE:O    | 1:C:450:THR:HG23 | 1.94                     | 0.68              |
| 1:D:370:LYS:HE2  | 1:D:370:LYS:HA   | 1.74                     | 0.68              |
| 1:A:315:ARG:HH11 | 1:A:315:ARG:HG3  | 1.60                     | 0.67              |
| 1:C:81:MET:HE3   | 1:C:514:MET:SD   | 2.34                     | 0.67              |
| 1:C:524:ALA:C    | 1:C:525:LYS:HD2  | 2.19                     | 0.67              |
| 1:F:125:ILE:HD13 | 1:F:517:ARG:HG2  | 1.77                     | 0.67              |
| 1:F:276:LEU:HD23 | 1:F:300:LEU:HB2  | 1.75                     | 0.67              |
| 1:H:82:MET:HE3   | 1:H:101:VAL:HG13 | 1.74                     | 0.67              |
| 1:E:189:LYS:HD2  | 1:E:189:LYS:C    | 2.19                     | 0.67              |
| 1:F:449:LYS:HE3  | 1:F:459:THR:HG21 | 1.76                     | 0.67              |
| 1:D:144:ILE:HD11 | 1:D:490:LEU:HD21 | 1.76                     | 0.67              |
| 1:E:425:TYR:O    | 1:E:429:VAL:HG23 | 1.94                     | 0.67              |
| 1:F:447:ILE:HB   | 1:F:448:PRO:HD3  | 1.76                     | 0.67              |
| 1:G:217:ARG:HB3  | 1:G:217:ARG:NH1  | 2.09                     | 0.67              |
| 1:G:315:ARG:HG3  | 1:G:315:ARG:HH11 | 1.59                     | 0.67              |
| 1:D:260:THR:H    | 1:D:264:GLN:HE21 | 1.40                     | 0.67              |
| 1:H:38:THR:O     | 1:H:50:LYS:HE3   | 1.95                     | 0.67              |
| 1:H:91:LYS:HB2   | 1:H:91:LYS:NZ    | 2.10                     | 0.67              |
| 1:C:150:ASP:OD2  | 1:C:152:GLU:HB3  | 1.94                     | 0.67              |
| 1:E:45:PRO:HA    | 1:E:164:GLY:HA2  | 1.75                     | 0.67              |
| 1:E:206:ALA:HA   | 1:E:384:ILE:HD11 | 1.76                     | 0.67              |
| 1:F:513:ILE:O    | 1:F:517:ARG:HG3  | 1.94                     | 0.67              |
| 1:H:157:ILE:HG13 | 1:H:401:VAL:HG21 | 1.77                     | 0.67              |
| 1:B:208:GLU:HB3  | 1:B:212:GLU:HG3  | 1.75                     | 0.67              |
| 1:D:11:ILE:C     | 1:D:11:ILE:HD13  | 2.20                     | 0.67              |
| 1:D:244:GLU:OE1  | 1:D:336:VAL:HG22 | 1.95                     | 0.67              |
| 1:E:469:GLU:HB2  | 1:E:477:ILE:HG21 | 1.77                     | 0.67              |
| 1:F:166:ASN:HA   | 1:G:517:ARG:NH1  | 2.10                     | 0.67              |
| 1:H:265:LEU:O    | 1:H:269:LEU:HD13 | 1.95                     | 0.67              |
| 1:A:60:VAL:HG21  | 1:A:71:LYS:HE2   | 1.77                     | 0.67              |
| 1:E:10:VAL:HG22  | 1:E:11:ILE:N     | 1.98                     | 0.67              |
| 1:G:348:GLU:O    | 1:G:349:VAL:HG23 | 1.93                     | 0.67              |
| 1:G:418:LEU:O    | 1:G:422:LEU:HB2  | 1.95                     | 0.67              |
| 1:D:272:GLU:HA   | 1:D:275:MET:HE3  | 1.76                     | 0.66              |
| 1:E:35:ILE:HD11  | 1:E:74:LEU:HD21  | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:227:HIS:HB3  | 1:G:230:MET:HG3  | 1.76                     | 0.66              |
| 1:A:150:ASP:OD2  | 1:A:152:GLU:HB3  | 1.95                     | 0.66              |
| 1:B:59:ILE:HD12  | 1:B:59:ILE:N     | 2.10                     | 0.66              |
| 1:B:409:PRO:HB3  | 1:B:490:LEU:HD11 | 1.76                     | 0.66              |
| 1:D:204:LYS:HD3  | 1:D:388:GLU:OE2  | 1.96                     | 0.66              |
| 1:G:217:ARG:HB3  | 1:G:217:ARG:HH11 | 1.60                     | 0.66              |
| 1:G:335:ASN:OD1  | 1:G:337:LYS:HB2  | 1.95                     | 0.66              |
| 1:H:102:VAL:HG12 | 1:H:446:ILE:HD13 | 1.77                     | 0.66              |
| 1:E:412:GLY:O    | 1:E:416:ILE:HG13 | 1.96                     | 0.66              |
| 1:A:257:ILE:HB   | 1:B:255:ALA:HB2  | 1.78                     | 0.66              |
| 1:H:125:ILE:HD13 | 1:H:517:ARG:HG2  | 1.76                     | 0.66              |
| 1:E:94:GLY:HA3   | 1:E:396:LYS:HD2  | 1.77                     | 0.66              |
| 1:G:29:ILE:O     | 1:G:33:ARG:HG3   | 1.96                     | 0.66              |
| 1:H:37:GLU:HG2   | 1:H:40:ARG:NH1   | 2.10                     | 0.66              |
| 1:A:109:ARG:NH2  | 1:A:110:LYS:HD3  | 2.10                     | 0.66              |
| 1:A:483:GLU:HG3  | 1:A:485:LYS:NZ   | 2.09                     | 0.66              |
| 1:H:35:ILE:HD11  | 1:H:74:LEU:HD21  | 1.78                     | 0.66              |
| 1:A:469:GLU:CB   | 1:A:477:ILE:HG21 | 2.25                     | 0.66              |
| 1:B:462:MET:O    | 1:B:466:VAL:HG23 | 1.95                     | 0.66              |
| 1:B:524:ALA:C    | 1:B:525:LYS:HD2  | 2.21                     | 0.66              |
| 1:C:272:GLU:HA   | 1:C:275:MET:HE3  | 1.78                     | 0.66              |
| 1:A:443:ALA:O    | 1:A:446:ILE:HG13 | 1.94                     | 0.66              |
| 1:C:142:ILE:HB   | 1:C:475:LEU:CD2  | 2.26                     | 0.66              |
| 1:D:197:LEU:HD22 | 1:D:395:VAL:HG12 | 1.78                     | 0.66              |
| 1:E:59:ILE:N     | 1:E:59:ILE:HD12  | 2.11                     | 0.66              |
| 1:F:126:LYS:NZ   | 1:F:126:LYS:HB3  | 2.10                     | 0.66              |
| 1:E:370:LYS:HA   | 1:E:370:LYS:HE2  | 1.77                     | 0.65              |
| 1:H:81:MET:HE3   | 1:H:514:MET:SD   | 2.36                     | 0.65              |
| 1:D:91:LYS:HB2   | 1:D:91:LYS:HZ2   | 1.59                     | 0.65              |
| 1:E:94:GLY:CA    | 1:E:396:LYS:HD2  | 2.25                     | 0.65              |
| 1:F:311:MET:HE1  | 1:F:350:VAL:HG12 | 1.78                     | 0.65              |
| 1:H:261:SER:O    | 1:H:264:GLN:HG3  | 1.95                     | 0.65              |
| 1:B:94:GLY:HA3   | 1:B:396:LYS:HD2  | 1.77                     | 0.65              |
| 1:B:413:ALA:HB3  | 1:B:414:PRO:HD3  | 1.78                     | 0.65              |
| 1:E:383:VAL:O    | 1:E:387:VAL:HG23 | 1.95                     | 0.65              |
| 1:H:380:THR:HG23 | 1:H:383:VAL:H    | 1.62                     | 0.65              |
| 1:D:206:ALA:HA   | 1:D:384:ILE:HD11 | 1.76                     | 0.65              |
| 1:D:445:LYS:O    | 1:D:448:PRO:HD2  | 1.95                     | 0.65              |
| 1:E:307:LYS:HD2  | 1:F:338:ASP:OD2  | 1.97                     | 0.65              |
| 1:G:145:ARG:HG2  | 1:G:145:ARG:HH11 | 1.61                     | 0.65              |
| 1:B:445:LYS:O    | 1:B:449:LYS:HB2  | 1.96                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:11:ILE:HD13  | 1:C:11:ILE:C     | 2.21                     | 0.65              |
| 1:D:446:ILE:O    | 1:D:450:THR:HG23 | 1.95                     | 0.65              |
| 1:A:517:ARG:HH12 | 1:H:166:ASN:HA   | 1.61                     | 0.65              |
| 1:B:380:THR:CG2  | 1:B:383:VAL:H    | 2.08                     | 0.65              |
| 1:C:271:GLN:HG3  | 1:C:275:MET:HE2  | 1.77                     | 0.65              |
| 1:B:188:LYS:HB2  | 1:B:193:TYR:HA   | 1.79                     | 0.65              |
| 1:D:524:ALA:O    | 1:D:525:LYS:HG2  | 1.97                     | 0.65              |
| 1:E:380:THR:HG22 | 1:E:383:VAL:CG2  | 2.14                     | 0.65              |
| 1:A:311:MET:HE1  | 1:A:350:VAL:HG12 | 1.77                     | 0.65              |
| 1:A:517:ARG:NH1  | 1:H:166:ASN:HA   | 2.11                     | 0.65              |
| 1:B:108:LEU:HD11 | 1:B:515:ILE:HD12 | 1.79                     | 0.65              |
| 1:C:155:LEU:HD13 | 1:C:179:VAL:HG21 | 1.78                     | 0.65              |
| 1:E:73:ASP:O     | 1:F:13:PRO:HD3   | 1.97                     | 0.65              |
| 1:F:258:ASN:HB3  | 1:G:258:ASN:HD21 | 1.61                     | 0.65              |
| 1:F:272:GLU:HA   | 1:F:275:MET:CE   | 2.26                     | 0.65              |
| 1:G:271:GLN:HG3  | 1:G:275:MET:HE2  | 1.78                     | 0.65              |
| 1:C:108:LEU:HD11 | 1:C:515:ILE:HD12 | 1.77                     | 0.65              |
| 1:G:462:MET:HE1  | 1:G:486:PRO:HD3  | 1.78                     | 0.65              |
| 1:C:10:VAL:CG2   | 1:C:11:ILE:H     | 2.05                     | 0.64              |
| 1:D:241:LEU:HD22 | 1:D:330:ALA:CB   | 2.27                     | 0.64              |
| 1:D:304:TYR:O    | 1:D:308:TYR:HD1  | 1.80                     | 0.64              |
| 1:E:205:LYS:NZ   | 1:E:358:GLU:HG2  | 2.12                     | 0.64              |
| 1:E:394:ALA:O    | 1:E:398:VAL:HG23 | 1.96                     | 0.64              |
| 1:C:166:ASN:HA   | 1:D:517:ARG:NH1  | 2.12                     | 0.64              |
| 1:F:297:ILE:HG22 | 1:F:302:GLN:HG3  | 1.79                     | 0.64              |
| 1:G:11:ILE:HG23  | 1:G:12:LEU:N     | 2.12                     | 0.64              |
| 1:B:166:ASN:HD22 | 1:B:166:ASN:C    | 2.05                     | 0.64              |
| 1:C:123:ILE:HG21 | 1:C:432:LYS:HB3  | 1.79                     | 0.64              |
| 1:G:37:GLU:HG2   | 1:G:40:ARG:NH1   | 2.12                     | 0.64              |
| 1:A:208:GLU:HB3  | 1:A:212:GLU:HG3  | 1.77                     | 0.64              |
| 1:D:138:ILE:HD13 | 1:D:421:ARG:HG2  | 1.79                     | 0.64              |
| 1:D:465:LYS:O    | 1:D:469:GLU:HG2  | 1.97                     | 0.64              |
| 1:A:126:LYS:NZ   | 1:A:126:LYS:HB3  | 2.11                     | 0.64              |
| 1:B:466:VAL:HG21 | 1:B:479:ILE:HG12 | 1.80                     | 0.64              |
| 1:D:226:VAL:HG12 | 1:D:312:ALA:O    | 1.97                     | 0.64              |
| 1:E:99:THR:O     | 1:E:103:ILE:HG13 | 1.97                     | 0.64              |
| 1:F:125:ILE:HG23 | 1:F:513:ILE:CG2  | 2.27                     | 0.64              |
| 1:H:372:VAL:HG22 | 1:H:373:THR:N    | 2.12                     | 0.64              |
| 1:C:461:GLU:HG2  | 1:C:465:LYS:HZ2  | 1.62                     | 0.64              |
| 1:F:204:LYS:HD3  | 1:F:388:GLU:OE2  | 1.98                     | 0.64              |
| 1:H:409:PRO:HB3  | 1:H:490:LEU:HD13 | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:311:MET:HE1  | 1:A:350:VAL:CG1  | 2.27                     | 0.64              |
| 1:D:211:GLU:OE1  | 1:D:211:GLU:HA   | 1.98                     | 0.64              |
| 1:E:293:VAL:CG2  | 1:E:297:ILE:HD11 | 2.25                     | 0.64              |
| 1:A:217:ARG:HB3  | 1:A:217:ARG:NH1  | 2.12                     | 0.63              |
| 1:E:261:SER:H    | 1:E:264:GLN:HE21 | 1.45                     | 0.63              |
| 1:F:225:VAL:HG21 | 1:F:232:LYS:HD3  | 1.80                     | 0.63              |
| 1:G:423:ASP:OD1  | 1:G:427:LYS:HE2  | 1.98                     | 0.63              |
| 1:A:30:LEU:O     | 1:A:34:ILE:HG13  | 1.98                     | 0.63              |
| 1:D:11:ILE:HD13  | 1:D:12:LEU:HB2   | 1.80                     | 0.63              |
| 1:E:447:ILE:HB   | 1:E:448:PRO:HD3  | 1.80                     | 0.63              |
| 1:F:123:ILE:HG21 | 1:F:432:LYS:HB3  | 1.79                     | 0.63              |
| 1:G:81:MET:HE3   | 1:G:514:MET:SD   | 2.38                     | 0.63              |
| 1:A:257:ILE:HG22 | 1:A:259:ILE:HD12 | 1.80                     | 0.63              |
| 1:A:445:LYS:O    | 1:A:449:LYS:HB2  | 1.98                     | 0.63              |
| 1:B:483:GLU:HG3  | 1:B:485:LYS:NZ   | 2.13                     | 0.63              |
| 1:D:447:ILE:HB   | 1:D:448:PRO:HD3  | 1.79                     | 0.63              |
| 1:H:383:VAL:O    | 1:H:387:VAL:HG23 | 1.98                     | 0.63              |
| 1:B:60:VAL:HG21  | 1:B:71:LYS:HE2   | 1.78                     | 0.63              |
| 1:F:235:GLU:HA   | 1:F:235:GLU:OE2  | 1.99                     | 0.63              |
| 1:F:269:LEU:HD12 | 1:G:251:THR:CG2  | 2.28                     | 0.63              |
| 1:E:227:HIS:ND1  | 1:E:228:PRO:HD2  | 2.13                     | 0.63              |
| 1:F:277:LYS:HB2  | 1:F:304:TYR:CE2  | 2.33                     | 0.63              |
| 1:B:29:ILE:O     | 1:B:33:ARG:HG3   | 1.98                     | 0.63              |
| 1:C:142:ILE:HB   | 1:C:475:LEU:HD22 | 1.79                     | 0.63              |
| 1:G:205:LYS:HZ3  | 1:G:358:GLU:HG2  | 1.63                     | 0.63              |
| 1:G:463:LEU:O    | 1:G:467:ILE:HG13 | 1.99                     | 0.63              |
| 1:E:166:ASN:HA   | 1:F:517:ARG:HH12 | 1.62                     | 0.63              |
| 1:E:513:ILE:O    | 1:E:517:ARG:HG3  | 1.99                     | 0.63              |
| 1:G:423:ASP:O    | 1:G:426:ALA:HB3  | 1.98                     | 0.63              |
| 1:A:85:VAL:HG13  | 1:A:507:SER:HB3  | 1.81                     | 0.63              |
| 1:E:29:ILE:O     | 1:E:33:ARG:HG3   | 1.98                     | 0.63              |
| 1:E:196:ASP:OD1  | 1:E:198:ASP:HB2  | 1.99                     | 0.63              |
| 1:E:212:GLU:HB2  | 1:E:377:ARG:HG3  | 1.81                     | 0.63              |
| 1:E:297:ILE:HG22 | 1:E:302:GLN:HG3  | 1.80                     | 0.63              |
| 1:F:188:LYS:HD3  | 1:F:193:TYR:CE1  | 2.34                     | 0.63              |
| 1:F:30:LEU:O     | 1:F:34:ILE:HG13  | 1.99                     | 0.62              |
| 1:A:125:ILE:HG23 | 1:A:513:ILE:CG2  | 2.27                     | 0.62              |
| 1:A:217:ARG:HB3  | 1:A:217:ARG:HH11 | 1.62                     | 0.62              |
| 1:B:145:ARG:HG2  | 1:B:145:ARG:NH1  | 2.11                     | 0.62              |
| 1:B:311:MET:HE1  | 1:B:350:VAL:CG1  | 2.29                     | 0.62              |
| 1:C:513:ILE:O    | 1:C:517:ARG:HG3  | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:10:VAL:HG13  | 1:G:11:ILE:N     | 2.10                     | 0.62              |
| 1:A:463:LEU:O    | 1:A:467:ILE:HG13 | 1.99                     | 0.62              |
| 1:B:166:ASN:HA   | 1:C:517:ARG:NH1  | 2.13                     | 0.62              |
| 1:D:409:PRO:HB3  | 1:D:490:LEU:HD13 | 1.80                     | 0.62              |
| 1:E:445:LYS:O    | 1:E:449:LYS:HB2  | 1.99                     | 0.62              |
| 1:F:383:VAL:O    | 1:F:387:VAL:HG23 | 1.99                     | 0.62              |
| 1:C:483:GLU:HG3  | 1:C:485:LYS:HZ1  | 1.65                     | 0.62              |
| 1:C:497:PRO:HB2  | 1:C:500:VAL:HG23 | 1.80                     | 0.62              |
| 1:E:265:LEU:O    | 1:E:269:LEU:HD13 | 1.99                     | 0.62              |
| 1:F:233:ARG:NH1  | 1:F:349:VAL:HG13 | 2.14                     | 0.62              |
| 1:C:22:ARG:HG3   | 1:C:23:ASP:N     | 2.14                     | 0.62              |
| 1:F:335:ASN:OD1  | 1:F:337:LYS:HB2  | 1.99                     | 0.62              |
| 1:G:465:LYS:O    | 1:G:469:GLU:HG2  | 1.99                     | 0.62              |
| 1:G:497:PRO:HB2  | 1:G:500:VAL:HG23 | 1.81                     | 0.62              |
| 1:A:59:ILE:HD12  | 1:A:59:ILE:N     | 2.15                     | 0.62              |
| 1:G:204:LYS:HD2  | 1:G:384:ILE:HG22 | 1.81                     | 0.62              |
| 1:G:354:LYS:HA   | 1:G:358:GLU:O    | 2.00                     | 0.62              |
| 1:H:64:ASP:O     | 1:H:68:ILE:HG13  | 1.99                     | 0.62              |
| 1:D:109:ARG:NH2  | 1:D:110:LYS:HD3  | 2.13                     | 0.62              |
| 1:G:188:LYS:HG3  | 1:G:192:LYS:C    | 2.24                     | 0.62              |
| 1:H:281:ASP:OD1  | 1:H:308:TYR:OH   | 2.13                     | 0.62              |
| 1:F:146:VAL:HG22 | 1:F:147:ASP:N    | 2.15                     | 0.62              |
| 1:F:286:THR:HG21 | 1:F:339:LEU:HG   | 1.82                     | 0.62              |
| 1:H:82:MET:HE1   | 1:H:104:ALA:HB3  | 1.80                     | 0.62              |
| 1:A:125:ILE:HD13 | 1:A:517:ARG:HG2  | 1.82                     | 0.62              |
| 1:A:257:ILE:HB   | 1:B:255:ALA:CB   | 2.30                     | 0.62              |
| 1:D:179:VAL:O    | 1:D:183:LYS:HG3  | 2.00                     | 0.62              |
| 1:D:404:ASP:OD1  | 1:D:499:ARG:HB2  | 1.99                     | 0.62              |
| 1:D:416:ILE:HD13 | 1:D:466:VAL:HG12 | 1.81                     | 0.62              |
| 1:E:17:GLN:NE2   | 1:E:17:GLN:H     | 1.97                     | 0.62              |
| 1:A:409:PRO:HB3  | 1:A:490:LEU:HD13 | 1.81                     | 0.61              |
| 1:C:204:LYS:HD3  | 1:C:388:GLU:OE2  | 1.99                     | 0.61              |
| 1:C:265:LEU:O    | 1:C:269:LEU:HD13 | 2.00                     | 0.61              |
| 1:E:73:ASP:HB3   | 1:F:13:PRO:HG2   | 1.82                     | 0.61              |
| 1:F:394:ALA:O    | 1:F:398:VAL:HG23 | 2.00                     | 0.61              |
| 1:G:388:GLU:O    | 1:G:392:GLU:HG3  | 1.99                     | 0.61              |
| 1:H:388:GLU:O    | 1:H:392:GLU:HG3  | 1.99                     | 0.61              |
| 1:B:150:ASP:OD1  | 1:B:153:THR:HG23 | 1.99                     | 0.61              |
| 1:B:509:SER:O    | 1:B:513:ILE:HG13 | 2.00                     | 0.61              |
| 1:F:413:ALA:HB3  | 1:F:414:PRO:HD3  | 1.81                     | 0.61              |
| 1:A:145:ARG:HG2  | 1:A:145:ARG:HH11 | 1.65                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:13:PRO:O     | 1:B:16:THR:HB    | 2.00                     | 0.61              |
| 1:C:11:ILE:HD13  | 1:C:11:ILE:O     | 2.00                     | 0.61              |
| 1:C:21:GLY:O     | 1:C:25:GLN:HG3   | 2.01                     | 0.61              |
| 1:H:189:LYS:HD2  | 1:H:189:LYS:C    | 2.25                     | 0.61              |
| 1:E:483:GLU:HG3  | 1:E:485:LYS:HZ3  | 1.64                     | 0.61              |
| 1:B:447:ILE:HB   | 1:B:448:PRO:HD3  | 1.82                     | 0.61              |
| 1:D:142:ILE:HB   | 1:D:475:LEU:HD22 | 1.81                     | 0.61              |
| 1:E:144:ILE:HD11 | 1:E:490:LEU:HD21 | 1.82                     | 0.61              |
| 1:A:11:ILE:HD11  | 1:H:31:ALA:HA    | 1.82                     | 0.61              |
| 1:H:175:ALA:O    | 1:H:179:VAL:HG23 | 2.01                     | 0.61              |
| 1:D:17:GLN:NE2   | 1:D:17:GLN:H     | 1.99                     | 0.61              |
| 1:E:388:GLU:O    | 1:E:392:GLU:HG3  | 2.00                     | 0.61              |
| 1:F:409:PRO:HB3  | 1:F:490:LEU:CD1  | 2.29                     | 0.61              |
| 1:F:445:LYS:O    | 1:F:448:PRO:HD2  | 2.01                     | 0.61              |
| 1:H:117:GLN:O    | 1:H:118:ASN:HB2  | 1.99                     | 0.61              |
| 1:H:311:MET:HE1  | 1:H:350:VAL:CG1  | 2.30                     | 0.61              |
| 1:C:260:THR:N    | 1:C:264:GLN:HE21 | 1.86                     | 0.61              |
| 1:D:106:GLU:HG2  | 1:D:446:ILE:CG1  | 2.31                     | 0.61              |
| 1:E:125:ILE:HD13 | 1:E:517:ARG:HG2  | 1.82                     | 0.61              |
| 1:E:151:GLU:O    | 1:E:155:LEU:HD23 | 2.01                     | 0.61              |
| 1:H:125:ILE:HG23 | 1:H:513:ILE:CG2  | 2.27                     | 0.61              |
| 1:H:126:LYS:NZ   | 1:H:126:LYS:HB3  | 2.16                     | 0.61              |
| 1:B:120:HIS:ND1  | 1:B:121:PRO:HD2  | 2.15                     | 0.61              |
| 1:E:60:VAL:HG21  | 1:E:71:LYS:HE2   | 1.83                     | 0.61              |
| 1:E:69:LEU:HB3   | 1:E:83:VAL:HG22  | 1.83                     | 0.61              |
| 1:G:348:GLU:HB3  | 1:G:365:GLY:HA3  | 1.82                     | 0.61              |
| 1:C:354:LYS:HE2  | 1:C:357:GLY:HA2  | 1.82                     | 0.60              |
| 1:C:445:LYS:O    | 1:C:449:LYS:HB2  | 2.01                     | 0.60              |
| 1:E:108:LEU:HD11 | 1:E:515:ILE:HD12 | 1.82                     | 0.60              |
| 1:B:103:ILE:O    | 1:B:107:LEU:HB2  | 2.00                     | 0.60              |
| 1:D:82:MET:HE3   | 1:D:101:VAL:HG13 | 1.82                     | 0.60              |
| 1:D:241:LEU:CD2  | 1:D:330:ALA:HB3  | 2.31                     | 0.60              |
| 1:F:106:GLU:HG2  | 1:F:446:ILE:CG1  | 2.31                     | 0.60              |
| 1:E:354:LYS:HE2  | 1:E:357:GLY:HA2  | 1.83                     | 0.60              |
| 1:F:81:MET:HE3   | 1:F:514:MET:SD   | 2.41                     | 0.60              |
| 1:F:243:ASN:OD1  | 1:F:295:LYS:HE3  | 2.00                     | 0.60              |
| 1:A:106:GLU:HG2  | 1:A:446:ILE:HG13 | 1.82                     | 0.60              |
| 1:B:261:SER:O    | 1:B:264:GLN:HB2  | 2.00                     | 0.60              |
| 1:D:469:GLU:CB   | 1:D:477:ILE:HG21 | 2.31                     | 0.60              |
| 1:F:197:LEU:HD22 | 1:F:395:VAL:CG1  | 2.31                     | 0.60              |
| 1:F:208:GLU:HB3  | 1:F:212:GLU:HG3  | 1.81                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:235:GLU:O    | 1:F:237:ALA:N    | 2.34                     | 0.60              |
| 1:G:126:LYS:HB3  | 1:G:126:LYS:NZ   | 2.17                     | 0.60              |
| 1:G:466:VAL:HG21 | 1:G:479:ILE:HG12 | 1.83                     | 0.60              |
| 1:H:155:LEU:HD22 | 1:H:179:VAL:HG21 | 1.84                     | 0.60              |
| 1:C:157:ILE:HG13 | 1:C:401:VAL:HG21 | 1.83                     | 0.60              |
| 1:F:244:GLU:OE1  | 1:F:336:VAL:HG22 | 2.01                     | 0.60              |
| 1:H:227:HIS:HD1  | 1:H:229:ARG:H    | 1.48                     | 0.60              |
| 1:C:269:LEU:HD12 | 1:D:251:THR:HG23 | 1.83                     | 0.60              |
| 1:D:151:GLU:O    | 1:D:155:LEU:HD23 | 2.02                     | 0.60              |
| 1:D:311:MET:HE1  | 1:D:350:VAL:CG1  | 2.32                     | 0.60              |
| 1:E:109:ARG:HG2  | 1:E:109:ARG:HH11 | 1.67                     | 0.60              |
| 1:A:179:VAL:O    | 1:A:183:LYS:HG3  | 2.02                     | 0.60              |
| 1:A:261:SER:H    | 1:A:264:GLN:HG3  | 1.66                     | 0.60              |
| 1:A:480:ASP:HB2  | 1:A:489:MET:HE1  | 1.83                     | 0.60              |
| 1:B:233:ARG:HD2  | 1:B:351:GLU:OE2  | 2.02                     | 0.60              |
| 1:D:217:ARG:HB3  | 1:D:217:ARG:HH11 | 1.66                     | 0.60              |
| 1:G:269:LEU:HD12 | 1:H:251:THR:HG23 | 1.84                     | 0.60              |
| 1:G:430:GLY:HA2  | 1:G:434:ALA:HB2  | 1.83                     | 0.60              |
| 1:F:157:ILE:HG13 | 1:F:401:VAL:HG21 | 1.84                     | 0.60              |
| 1:B:241:LEU:HD12 | 1:B:292:PHE:HB2  | 1.83                     | 0.60              |
| 1:A:77:PRO:HB2   | 1:H:51:MET:CE    | 2.31                     | 0.59              |
| 1:A:209:GLY:C    | 1:A:211:GLU:N    | 2.60                     | 0.59              |
| 1:C:59:ILE:N     | 1:C:59:ILE:HD12  | 2.17                     | 0.59              |
| 1:C:64:ASP:O     | 1:C:68:ILE:HG13  | 2.02                     | 0.59              |
| 1:H:260:THR:N    | 1:H:264:GLN:NE2  | 2.44                     | 0.59              |
| 1:H:465:LYS:O    | 1:H:469:GLU:HG2  | 2.01                     | 0.59              |
| 1:B:182:VAL:O    | 1:B:186:ALA:HB2  | 2.03                     | 0.59              |
| 1:B:348:GLU:HB3  | 1:B:365:GLY:HA3  | 1.84                     | 0.59              |
| 1:C:261:SER:O    | 1:C:264:GLN:HG3  | 2.02                     | 0.59              |
| 1:E:142:ILE:HB   | 1:E:475:LEU:HD22 | 1.82                     | 0.59              |
| 1:F:175:ALA:O    | 1:F:179:VAL:HG23 | 2.02                     | 0.59              |
| 1:A:197:LEU:HD22 | 1:A:395:VAL:CG1  | 2.31                     | 0.59              |
| 1:C:117:GLN:O    | 1:C:118:ASN:HB2  | 2.01                     | 0.59              |
| 1:H:59:ILE:N     | 1:H:59:ILE:HD12  | 2.16                     | 0.59              |
| 1:H:136:GLN:NE2  | 1:H:136:GLN:HA   | 2.17                     | 0.59              |
| 1:H:211:GLU:OE1  | 1:H:211:GLU:HA   | 2.00                     | 0.59              |
| 1:A:475:LEU:HD12 | 1:A:475:LEU:O    | 2.03                     | 0.59              |
| 1:C:205:LYS:O    | 1:C:377:ARG:NH1  | 2.35                     | 0.59              |
| 1:E:443:ALA:O    | 1:E:446:ILE:HG13 | 2.03                     | 0.59              |
| 1:F:22:ARG:HG3   | 1:F:23:ASP:N     | 2.18                     | 0.59              |
| 1:F:206:ALA:HA   | 1:F:384:ILE:HD11 | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:136:GLN:HA   | 1:G:136:GLN:HE21 | 1.67                     | 0.59              |
| 1:E:106:GLU:HG2  | 1:E:446:ILE:CG1  | 2.33                     | 0.59              |
| 1:E:145:ARG:HG2  | 1:E:145:ARG:HH11 | 1.67                     | 0.59              |
| 1:H:418:LEU:O    | 1:H:422:LEU:HB2  | 2.03                     | 0.59              |
| 1:B:216:VAL:O    | 1:B:372:VAL:HG23 | 2.02                     | 0.59              |
| 1:B:230:MET:HE1  | 1:B:312:ALA:HB3  | 1.84                     | 0.59              |
| 1:D:348:GLU:O    | 1:D:349:VAL:HG23 | 2.02                     | 0.59              |
| 1:A:265:LEU:O    | 1:A:269:LEU:HD13 | 2.02                     | 0.59              |
| 1:A:423:ASP:O    | 1:A:426:ALA:HB3  | 2.02                     | 0.59              |
| 1:D:418:LEU:O    | 1:D:422:LEU:HB2  | 2.03                     | 0.59              |
| 1:E:271:GLN:O    | 1:E:275:MET:HG3  | 2.02                     | 0.59              |
| 1:E:272:GLU:HA   | 1:E:275:MET:CE   | 2.27                     | 0.59              |
| 1:F:257:ILE:HG22 | 1:F:259:ILE:HD12 | 1.85                     | 0.59              |
| 1:F:465:LYS:O    | 1:F:469:GLU:HG2  | 2.03                     | 0.59              |
| 1:A:12:LEU:HD13  | 1:A:16:THR:HG21  | 1.83                     | 0.59              |
| 1:A:235:GLU:O    | 1:A:236:ASN:C    | 2.45                     | 0.59              |
| 1:D:172:GLU:OE1  | 1:D:172:GLU:HA   | 2.01                     | 0.59              |
| 1:E:109:ARG:NH2  | 1:E:110:LYS:HD3  | 2.17                     | 0.59              |
| 1:E:423:ASP:OD1  | 1:E:427:LYS:HE2  | 2.02                     | 0.59              |
| 1:A:466:VAL:HG21 | 1:A:479:ILE:HG12 | 1.85                     | 0.59              |
| 1:C:461:GLU:HG2  | 1:C:465:LYS:NZ   | 2.18                     | 0.59              |
| 1:G:126:LYS:O    | 1:G:130:LEU:HG   | 2.02                     | 0.59              |
| 1:G:353:ARG:NH2  | 1:G:364:GLU:OE2  | 2.35                     | 0.59              |
| 1:H:328:THR:HG22 | 1:H:366:CYS:SG   | 2.43                     | 0.59              |
| 1:H:509:SER:O    | 1:H:513:ILE:HG13 | 2.03                     | 0.59              |
| 1:A:450:THR:O    | 1:A:454:ASN:ND2  | 2.36                     | 0.59              |
| 1:C:433:GLU:O    | 1:C:437:ILE:HG13 | 2.02                     | 0.59              |
| 1:E:227:HIS:HB3  | 1:E:230:MET:CG   | 2.30                     | 0.59              |
| 1:G:205:LYS:NZ   | 1:G:358:GLU:HG2  | 2.17                     | 0.59              |
| 1:G:409:PRO:HB3  | 1:G:490:LEU:HD13 | 1.85                     | 0.59              |
| 1:B:445:LYS:C    | 1:B:448:PRO:HD2  | 2.28                     | 0.58              |
| 1:C:226:VAL:HG12 | 1:C:312:ALA:O    | 2.03                     | 0.58              |
| 1:D:182:VAL:O    | 1:D:186:ALA:HB2  | 2.03                     | 0.58              |
| 1:G:157:ILE:HG13 | 1:G:401:VAL:HG21 | 1.85                     | 0.58              |
| 1:G:276:LEU:HD23 | 1:G:300:LEU:HB2  | 1.84                     | 0.58              |
| 1:A:209:GLY:C    | 1:A:211:GLU:H    | 2.10                     | 0.58              |
| 1:A:266:MET:O    | 1:A:270:GLU:HG3  | 2.02                     | 0.58              |
| 1:B:400:ASP:OD1  | 1:B:499:ARG:HD2  | 2.04                     | 0.58              |
| 1:C:82:MET:HE1   | 1:C:104:ALA:HB3  | 1.84                     | 0.58              |
| 1:E:167:ALA:C    | 1:E:169:SER:H    | 2.11                     | 0.58              |
| 1:G:170:HIS:CE1  | 1:G:210:VAL:HB   | 2.38                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:416:ILE:HD13 | 1:G:466:VAL:HG12 | 1.84                     | 0.58              |
| 1:H:120:HIS:ND1  | 1:H:122:SER:HB3  | 2.18                     | 0.58              |
| 1:D:106:GLU:HG2  | 1:D:446:ILE:HG13 | 1.83                     | 0.58              |
| 1:E:91:LYS:HG2   | 1:E:91:LYS:O     | 2.04                     | 0.58              |
| 1:G:513:ILE:O    | 1:G:517:ARG:HG3  | 2.03                     | 0.58              |
| 1:C:204:LYS:HD2  | 1:C:384:ILE:HG22 | 1.86                     | 0.58              |
| 1:D:315:ARG:HG3  | 1:D:315:ARG:NH1  | 2.19                     | 0.58              |
| 1:F:233:ARG:NH1  | 1:F:349:VAL:CG1  | 2.65                     | 0.58              |
| 1:H:264:GLN:HA   | 1:H:267:SER:OG   | 2.04                     | 0.58              |
| 1:B:189:LYS:HD2  | 1:B:189:LYS:C    | 2.28                     | 0.58              |
| 1:C:353:ARG:NH2  | 1:C:364:GLU:OE2  | 2.36                     | 0.58              |
| 1:F:150:ASP:OD1  | 1:F:153:THR:HG23 | 2.03                     | 0.58              |
| 1:F:271:GLN:O    | 1:F:275:MET:HG3  | 2.04                     | 0.58              |
| 1:B:297:ILE:HG22 | 1:B:302:GLN:HG3  | 1.84                     | 0.58              |
| 1:D:110:LYS:HE3  | 1:D:442:ASP:OD1  | 2.03                     | 0.58              |
| 1:G:445:LYS:O    | 1:G:448:PRO:HD2  | 2.04                     | 0.58              |
| 1:A:206:ALA:CA   | 1:A:384:ILE:HD11 | 2.32                     | 0.58              |
| 1:D:303:HIS:CD2  | 1:E:335:ASN:HB3  | 2.39                     | 0.58              |
| 1:D:409:PRO:HB3  | 1:D:490:LEU:CD1  | 2.33                     | 0.58              |
| 1:A:226:VAL:HG12 | 1:A:312:ALA:O    | 2.03                     | 0.58              |
| 1:D:480:ASP:HB2  | 1:D:489:MET:HE1  | 1.86                     | 0.58              |
| 1:F:11:ILE:HD13  | 1:F:11:ILE:C     | 2.29                     | 0.58              |
| 1:A:400:ASP:OD1  | 1:A:499:ARG:HD2  | 2.04                     | 0.58              |
| 1:D:188:LYS:HB2  | 1:D:193:TYR:HA   | 1.86                     | 0.58              |
| 1:F:96:GLY:HA2   | 3:F:6528:ADP:O1B | 2.04                     | 0.58              |
| 1:F:184:GLN:NE2  | 1:F:217:ARG:NH2  | 2.52                     | 0.58              |
| 1:F:469:GLU:HB2  | 1:F:477:ILE:HG21 | 1.85                     | 0.58              |
| 1:G:370:LYS:HA   | 1:G:370:LYS:CE   | 2.34                     | 0.58              |
| 1:H:216:VAL:O    | 1:H:218:GLY:N    | 2.36                     | 0.58              |
| 1:B:277:LYS:HD2  | 1:B:304:TYR:CE1  | 2.39                     | 0.57              |
| 1:B:513:ILE:O    | 1:B:517:ARG:HG3  | 2.02                     | 0.57              |
| 1:D:29:ILE:HG23  | 1:D:108:LEU:HB3  | 1.86                     | 0.57              |
| 1:D:280:VAL:HG13 | 1:D:305:LEU:HG   | 1.84                     | 0.57              |
| 1:A:276:LEU:HD23 | 1:A:300:LEU:HB2  | 1.86                     | 0.57              |
| 1:C:123:ILE:HG21 | 1:C:432:LYS:CB   | 2.34                     | 0.57              |
| 1:C:154:LEU:HD21 | 1:C:402:MET:HE3  | 1.85                     | 0.57              |
| 1:C:183:LYS:HG2  | 1:C:402:MET:HE1  | 1.85                     | 0.57              |
| 1:D:45:PRO:HA    | 1:D:164:GLY:HA2  | 1.85                     | 0.57              |
| 1:E:136:GLN:HA   | 1:E:136:GLN:NE2  | 2.18                     | 0.57              |
| 1:E:342:GLU:N    | 1:E:342:GLU:OE2  | 2.37                     | 0.57              |
| 1:F:233:ARG:HH12 | 1:F:349:VAL:HG13 | 1.65                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:29:ILE:HG23  | 1:A:108:LEU:HB3  | 1.86                     | 0.57              |
| 1:B:277:LYS:HB2  | 1:B:304:TYR:CE2  | 2.39                     | 0.57              |
| 1:C:120:HIS:ND1  | 1:C:122:SER:HB3  | 2.18                     | 0.57              |
| 1:D:466:VAL:HG22 | 1:D:486:PRO:HG3  | 1.86                     | 0.57              |
| 1:E:154:LEU:HG   | 1:E:398:VAL:HG13 | 1.86                     | 0.57              |
| 1:H:29:ILE:HG23  | 1:H:108:LEU:HB3  | 1.86                     | 0.57              |
| 1:A:158:ALA:O    | 1:A:162:ILE:HG13 | 2.04                     | 0.57              |
| 1:A:304:TYR:O    | 1:A:308:TYR:HD1  | 1.88                     | 0.57              |
| 1:A:393:ASP:O    | 1:A:397:VAL:HG22 | 2.05                     | 0.57              |
| 1:C:150:ASP:OD1  | 1:C:153:THR:HG23 | 2.04                     | 0.57              |
| 1:H:280:VAL:HG13 | 1:H:305:LEU:HG   | 1.86                     | 0.57              |
| 1:H:417:GLU:OE2  | 1:H:470:HIS:NE2  | 2.28                     | 0.57              |
| 1:B:126:LYS:HB3  | 1:B:126:LYS:NZ   | 2.19                     | 0.57              |
| 1:C:146:VAL:HG22 | 1:C:147:ASP:N    | 2.19                     | 0.57              |
| 1:E:509:SER:O    | 1:E:513:ILE:HG13 | 2.05                     | 0.57              |
| 1:A:189:LYS:HD2  | 1:A:189:LYS:C    | 2.28                     | 0.57              |
| 1:C:37:GLU:HG2   | 1:C:40:ARG:NH1   | 2.19                     | 0.57              |
| 1:C:445:LYS:C    | 1:C:448:PRO:HD2  | 2.30                     | 0.57              |
| 1:D:114:LEU:HD22 | 1:D:119:ILE:HD12 | 1.86                     | 0.57              |
| 1:E:82:MET:HE3   | 1:E:101:VAL:HG13 | 1.86                     | 0.57              |
| 1:F:497:PRO:HB2  | 1:F:500:VAL:HG23 | 1.86                     | 0.57              |
| 1:G:445:LYS:O    | 1:G:449:LYS:HB2  | 2.05                     | 0.57              |
| 1:H:462:MET:HA   | 1:H:462:MET:HE3  | 1.87                     | 0.57              |
| 1:A:38:THR:O     | 1:A:50:LYS:CE    | 2.52                     | 0.57              |
| 1:B:94:GLY:CA    | 1:B:396:LYS:HD2  | 2.34                     | 0.57              |
| 1:B:394:ALA:O    | 1:B:398:VAL:HG23 | 2.04                     | 0.57              |
| 1:D:388:GLU:O    | 1:D:392:GLU:HG3  | 2.05                     | 0.57              |
| 1:E:222:ASP:OD1  | 1:E:360:MET:HE3  | 2.04                     | 0.57              |
| 1:F:204:LYS:HD2  | 1:F:384:ILE:HG22 | 1.86                     | 0.57              |
| 1:G:11:ILE:CG2   | 1:G:12:LEU:N     | 2.67                     | 0.57              |
| 1:H:241:LEU:HD22 | 1:H:330:ALA:CB   | 2.35                     | 0.57              |
| 1:A:241:LEU:HD22 | 1:A:330:ALA:HB3  | 1.87                     | 0.57              |
| 1:B:12:LEU:HD21  | 1:B:16:THR:HG21  | 1.87                     | 0.57              |
| 1:B:227:HIS:HB3  | 1:B:230:MET:HG3  | 1.87                     | 0.57              |
| 1:B:412:GLY:O    | 1:B:415:GLU:HG2  | 2.05                     | 0.57              |
| 1:C:297:ILE:HG22 | 1:C:302:GLN:HG3  | 1.86                     | 0.57              |
| 1:C:425:TYR:O    | 1:C:429:VAL:HG23 | 2.05                     | 0.57              |
| 1:C:443:ALA:O    | 1:C:446:ILE:HG13 | 2.04                     | 0.57              |
| 1:D:259:ILE:HG22 | 1:E:257:ILE:HG23 | 1.85                     | 0.57              |
| 1:D:261:SER:H    | 1:D:264:GLN:HE21 | 1.52                     | 0.57              |
| 1:E:138:ILE:HD13 | 1:E:421:ARG:HG2  | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:412:GLY:O    | 1:E:415:GLU:HG2  | 2.05                     | 0.57              |
| 1:A:75:GLN:HB2   | 1:B:11:ILE:CA    | 2.35                     | 0.57              |
| 1:H:205:LYS:O    | 1:H:377:ARG:NH1  | 2.38                     | 0.57              |
| 1:A:37:GLU:HG2   | 1:A:40:ARG:NH1   | 2.20                     | 0.56              |
| 1:D:197:LEU:HD22 | 1:D:395:VAL:CG1  | 2.35                     | 0.56              |
| 1:F:59:ILE:HD12  | 1:F:59:ILE:N     | 2.20                     | 0.56              |
| 1:G:147:ASP:O    | 1:G:149:ASP:N    | 2.38                     | 0.56              |
| 1:G:261:SER:O    | 1:G:264:GLN:HG3  | 2.05                     | 0.56              |
| 1:A:509:SER:O    | 1:A:513:ILE:HG13 | 2.05                     | 0.56              |
| 1:F:13:PRO:O     | 1:F:16:THR:HB    | 2.05                     | 0.56              |
| 1:F:270:GLU:HA   | 1:F:273:GLU:HG3  | 1.86                     | 0.56              |
| 1:F:461:GLU:HG2  | 1:F:465:LYS:HZ2  | 1.71                     | 0.56              |
| 1:H:76:HIS:CD2   | 1:H:78:ALA:HB3   | 2.40                     | 0.56              |
| 1:H:125:ILE:CD1  | 1:H:517:ARG:HG2  | 2.34                     | 0.56              |
| 1:A:99:THR:O     | 1:A:103:ILE:HG13 | 2.04                     | 0.56              |
| 1:B:54:ASP:OD1   | 1:B:58:ASP:HB3   | 2.06                     | 0.56              |
| 1:B:91:LYS:HB2   | 1:B:91:LYS:NZ    | 2.20                     | 0.56              |
| 1:B:179:VAL:O    | 1:B:183:LYS:HG3  | 2.05                     | 0.56              |
| 1:B:197:LEU:HD22 | 1:B:395:VAL:CG1  | 2.35                     | 0.56              |
| 1:B:250:LYS:NZ   | 1:C:253:THR:HA   | 2.19                     | 0.56              |
| 1:B:462:MET:CE   | 1:B:486:PRO:HD3  | 2.35                     | 0.56              |
| 1:D:126:LYS:NZ   | 1:D:126:LYS:HB3  | 2.20                     | 0.56              |
| 1:D:147:ASP:HB3  | 1:D:150:ASP:HB2  | 1.88                     | 0.56              |
| 1:D:217:ARG:HH11 | 1:D:217:ARG:CB   | 2.17                     | 0.56              |
| 1:D:497:PRO:HB2  | 1:D:500:VAL:HG23 | 1.86                     | 0.56              |
| 1:F:134:LYS:O    | 1:F:138:ILE:HG13 | 2.05                     | 0.56              |
| 1:F:179:VAL:O    | 1:F:183:LYS:HG3  | 2.04                     | 0.56              |
| 1:F:272:GLU:HA   | 1:F:275:MET:HE3  | 1.87                     | 0.56              |
| 1:A:138:ILE:CD1  | 1:A:421:ARG:HG2  | 2.34                     | 0.56              |
| 1:C:413:ALA:HB3  | 1:C:414:PRO:HD3  | 1.87                     | 0.56              |
| 1:E:150:ASP:OD2  | 1:E:152:GLU:HB3  | 2.05                     | 0.56              |
| 1:E:266:MET:HG2  | 1:F:271:GLN:NE2  | 2.20                     | 0.56              |
| 1:F:123:ILE:HG21 | 1:F:432:LYS:CB   | 2.35                     | 0.56              |
| 1:F:204:LYS:HB3  | 1:F:384:ILE:HG21 | 1.87                     | 0.56              |
| 1:F:210:VAL:HA   | 1:F:377:ARG:O    | 2.05                     | 0.56              |
| 1:G:51:MET:HB2   | 1:H:518:ILE:HD13 | 1.86                     | 0.56              |
| 1:G:64:ASP:O     | 1:G:68:ILE:HG13  | 2.05                     | 0.56              |
| 1:A:182:VAL:O    | 1:A:186:ALA:HB2  | 2.06                     | 0.56              |
| 1:C:409:PRO:HB3  | 1:C:490:LEU:HD12 | 1.88                     | 0.56              |
| 1:D:513:ILE:O    | 1:D:517:ARG:HG3  | 2.05                     | 0.56              |
| 1:F:458:ASP:O    | 1:F:459:THR:C    | 2.48                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:348:GLU:O    | 1:H:349:VAL:HG23 | 2.06                     | 0.56              |
| 1:F:184:GLN:HE22 | 1:F:217:ARG:HH21 | 1.54                     | 0.56              |
| 1:A:272:GLU:HA   | 1:A:275:MET:HE3  | 1.87                     | 0.56              |
| 1:B:241:LEU:CD2  | 1:B:330:ALA:HB3  | 2.35                     | 0.56              |
| 1:C:257:ILE:HG22 | 1:C:259:ILE:HD12 | 1.87                     | 0.56              |
| 1:D:175:ALA:O    | 1:D:179:VAL:HG23 | 2.06                     | 0.56              |
| 1:D:226:VAL:HG22 | 1:D:302:GLN:OE1  | 2.06                     | 0.56              |
| 1:E:233:ARG:HH11 | 1:E:233:ARG:HG3  | 1.71                     | 0.56              |
| 1:G:196:ASP:OD1  | 1:G:198:ASP:HB2  | 2.06                     | 0.56              |
| 1:B:276:LEU:HD23 | 1:B:300:LEU:HB2  | 1.87                     | 0.56              |
| 1:D:75:GLN:HB2   | 1:E:10:VAL:C     | 2.31                     | 0.56              |
| 1:E:38:THR:O     | 1:E:50:LYS:HE3   | 2.06                     | 0.56              |
| 1:F:10:VAL:CG2   | 1:F:11:ILE:H     | 2.13                     | 0.56              |
| 1:F:483:GLU:HG3  | 1:F:485:LYS:NZ   | 2.21                     | 0.56              |
| 1:G:94:GLY:HA3   | 1:G:396:LYS:HD2  | 1.88                     | 0.56              |
| 1:C:151:GLU:O    | 1:C:155:LEU:HD23 | 2.06                     | 0.56              |
| 1:D:150:ASP:OD1  | 1:D:153:THR:HG23 | 2.06                     | 0.56              |
| 1:D:196:ASP:OD1  | 1:D:198:ASP:HB2  | 2.06                     | 0.56              |
| 1:D:209:GLY:C    | 1:D:211:GLU:H    | 2.11                     | 0.56              |
| 1:E:11:ILE:HD13  | 1:E:11:ILE:O     | 2.05                     | 0.56              |
| 1:E:218:GLY:HA3  | 1:E:363:VAL:O    | 2.06                     | 0.56              |
| 1:H:54:ASP:OD1   | 1:H:56:LEU:HB2   | 2.06                     | 0.56              |
| 1:D:10:VAL:CG2   | 1:D:11:ILE:H     | 2.08                     | 0.56              |
| 1:E:17:GLN:H     | 1:E:17:GLN:HE21  | 1.54                     | 0.56              |
| 1:E:266:MET:O    | 1:E:270:GLU:HG3  | 2.06                     | 0.56              |
| 1:F:146:VAL:HG22 | 1:F:147:ASP:H    | 1.70                     | 0.56              |
| 1:G:125:ILE:CD1  | 1:G:517:ARG:HG2  | 2.33                     | 0.56              |
| 1:A:230:MET:HE1  | 1:A:312:ALA:CB   | 2.30                     | 0.55              |
| 1:D:423:ASP:OD1  | 1:D:427:LYS:HE2  | 2.06                     | 0.55              |
| 1:E:372:VAL:HG22 | 1:E:373:THR:H    | 1.70                     | 0.55              |
| 1:E:450:THR:O    | 1:E:454:ASN:ND2  | 2.38                     | 0.55              |
| 1:G:315:ARG:HG3  | 1:G:315:ARG:NH1  | 2.20                     | 0.55              |
| 1:C:315:ARG:HG3  | 1:C:315:ARG:NH1  | 2.21                     | 0.55              |
| 1:D:501:LYS:HA   | 1:D:501:LYS:HE3  | 1.88                     | 0.55              |
| 1:F:348:GLU:HB3  | 1:F:365:GLY:HA3  | 1.88                     | 0.55              |
| 1:F:421:ARG:HH11 | 1:F:421:ARG:CB   | 2.11                     | 0.55              |
| 1:G:166:ASN:HA   | 1:H:517:ARG:NH1  | 2.19                     | 0.55              |
| 1:G:380:THR:HG22 | 1:G:383:VAL:CG2  | 2.26                     | 0.55              |
| 1:H:54:ASP:CB    | 1:H:58:ASP:HB3   | 2.33                     | 0.55              |
| 1:H:473:ARG:HB2  | 1:H:477:ILE:HG13 | 1.87                     | 0.55              |
| 1:B:204:LYS:HD2  | 1:B:384:ILE:HG22 | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:233:ARG:HH12 | 1:C:349:VAL:HG11 | 1.71                     | 0.55              |
| 1:D:462:MET:HA   | 1:D:462:MET:HE3  | 1.86                     | 0.55              |
| 1:G:208:GLU:HB3  | 1:G:212:GLU:CG   | 2.36                     | 0.55              |
| 1:A:211:GLU:OE1  | 1:A:211:GLU:HA   | 2.06                     | 0.55              |
| 1:E:197:LEU:HD22 | 1:E:395:VAL:CG1  | 2.36                     | 0.55              |
| 1:E:480:ASP:HB2  | 1:E:489:MET:HE1  | 1.89                     | 0.55              |
| 1:G:204:LYS:HB3  | 1:G:384:ILE:CG2  | 2.36                     | 0.55              |
| 1:E:123:ILE:HG21 | 1:E:432:LYS:HB3  | 1.89                     | 0.55              |
| 1:E:355:LEU:O    | 1:E:356:ALA:HB3  | 2.05                     | 0.55              |
| 1:E:400:ASP:O    | 1:E:404:ASP:HB2  | 2.07                     | 0.55              |
| 1:E:409:PRO:HB3  | 1:E:490:LEU:CD1  | 2.36                     | 0.55              |
| 1:F:208:GLU:HB3  | 1:F:212:GLU:CG   | 2.37                     | 0.55              |
| 1:G:30:LEU:O     | 1:G:34:ILE:HG13  | 2.07                     | 0.55              |
| 1:G:401:VAL:O    | 1:G:405:GLY:N    | 2.37                     | 0.55              |
| 1:D:483:GLU:HG3  | 1:D:485:LYS:NZ   | 2.22                     | 0.55              |
| 1:E:260:THR:H    | 1:E:264:GLN:HE22 | 1.53                     | 0.55              |
| 1:F:60:VAL:HG21  | 1:F:71:LYS:HE2   | 1.89                     | 0.55              |
| 1:G:443:ALA:O    | 1:G:446:ILE:HG13 | 2.06                     | 0.55              |
| 1:H:81:MET:HE1   | 1:H:515:ILE:HG12 | 1.87                     | 0.55              |
| 1:B:463:LEU:O    | 1:B:467:ILE:HG13 | 2.07                     | 0.55              |
| 1:C:423:ASP:OD1  | 1:C:427:LYS:HE2  | 2.07                     | 0.55              |
| 1:D:250:LYS:NZ   | 1:E:253:THR:HA   | 2.22                     | 0.55              |
| 1:D:293:VAL:CG2  | 1:D:297:ILE:HD11 | 2.36                     | 0.55              |
| 1:D:394:ALA:O    | 1:D:398:VAL:HG23 | 2.07                     | 0.55              |
| 1:E:412:GLY:HA2  | 1:E:415:GLU:OE2  | 2.06                     | 0.55              |
| 1:G:269:LEU:HD12 | 1:H:251:THR:CG2  | 2.37                     | 0.55              |
| 1:H:140:ASP:OD1  | 1:H:502:LYS:HD2  | 2.07                     | 0.55              |
| 1:H:210:VAL:HA   | 1:H:377:ARG:O    | 2.07                     | 0.55              |
| 1:B:241:LEU:HD22 | 1:B:330:ALA:HB3  | 1.88                     | 0.55              |
| 1:B:272:GLU:HA   | 1:B:275:MET:CE   | 2.33                     | 0.55              |
| 1:C:16:THR:HG23  | 1:C:523:ALA:O    | 2.06                     | 0.55              |
| 1:F:204:LYS:HB3  | 1:F:384:ILE:CG2  | 2.37                     | 0.55              |
| 1:F:235:GLU:O    | 1:F:236:ASN:C    | 2.50                     | 0.55              |
| 1:F:276:LEU:HD23 | 1:F:300:LEU:CB   | 2.36                     | 0.55              |
| 1:G:35:ILE:HG13  | 1:G:79:ALA:HB1   | 1.89                     | 0.55              |
| 1:G:128:TYR:CE2  | 1:G:440:PHE:HB2  | 2.42                     | 0.55              |
| 1:A:205:LYS:O    | 1:A:377:ARG:NH1  | 2.40                     | 0.55              |
| 1:D:392:GLU:O    | 1:D:396:LYS:HE3  | 2.07                     | 0.55              |
| 1:E:142:ILE:HB   | 1:E:475:LEU:CD2  | 2.37                     | 0.55              |
| 1:E:215:LEU:HD11 | 1:E:372:VAL:HG21 | 1.89                     | 0.55              |
| 1:F:272:GLU:HA   | 1:F:275:MET:HE2  | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:480:ASP:HB2  | 1:H:489:MET:HE1  | 1.89                     | 0.55              |
| 1:C:29:ILE:O     | 1:C:33:ARG:HG3   | 2.06                     | 0.54              |
| 1:C:136:GLN:NE2  | 1:C:136:GLN:HA   | 2.22                     | 0.54              |
| 1:C:290:VAL:HG22 | 1:C:311:MET:HE2  | 1.87                     | 0.54              |
| 1:G:125:ILE:HG23 | 1:G:513:ILE:CG2  | 2.37                     | 0.54              |
| 1:H:215:LEU:HD11 | 1:H:372:VAL:CG2  | 2.37                     | 0.54              |
| 1:A:286:THR:HG21 | 1:A:339:LEU:HG   | 1.90                     | 0.54              |
| 1:D:350:VAL:HG13 | 1:D:363:VAL:HG22 | 1.89                     | 0.54              |
| 1:F:196:ASP:OD1  | 1:F:198:ASP:HB2  | 2.06                     | 0.54              |
| 1:G:189:LYS:HD2  | 1:G:189:LYS:C    | 2.32                     | 0.54              |
| 1:G:311:MET:HE1  | 1:G:350:VAL:CG1  | 2.37                     | 0.54              |
| 1:H:11:ILE:HG23  | 1:H:12:LEU:H     | 1.72                     | 0.54              |
| 1:B:258:ASN:HB3  | 1:C:258:ASN:HD21 | 1.72                     | 0.54              |
| 1:C:227:HIS:HB3  | 1:C:230:MET:HG3  | 1.89                     | 0.54              |
| 1:D:238:LYS:HD2  | 1:D:287:GLY:O    | 2.08                     | 0.54              |
| 1:D:248:VAL:HG11 | 1:D:272:GLU:OE2  | 2.07                     | 0.54              |
| 1:D:466:VAL:HG21 | 1:D:479:ILE:HG12 | 1.89                     | 0.54              |
| 1:D:488:ASP:O    | 1:D:492:LYS:HG2  | 2.07                     | 0.54              |
| 1:F:461:GLU:HG2  | 1:F:465:LYS:NZ   | 2.22                     | 0.54              |
| 1:A:417:GLU:OE2  | 1:A:470:HIS:NE2  | 2.34                     | 0.54              |
| 1:B:209:GLY:O    | 1:B:212:GLU:HG2  | 2.07                     | 0.54              |
| 1:D:380:THR:HG23 | 1:D:383:VAL:H    | 1.72                     | 0.54              |
| 1:F:205:LYS:HZ2  | 1:F:360:MET:HE3  | 1.72                     | 0.54              |
| 1:G:217:ARG:HA   | 1:G:372:VAL:HG23 | 1.89                     | 0.54              |
| 1:G:370:LYS:HE2  | 1:G:370:LYS:CA   | 2.35                     | 0.54              |
| 1:A:260:THR:N    | 1:A:264:GLN:HE21 | 1.97                     | 0.54              |
| 1:A:461:GLU:HG2  | 1:A:465:LYS:HZ3  | 1.71                     | 0.54              |
| 1:C:75:GLN:HB2   | 1:D:11:ILE:C     | 2.32                     | 0.54              |
| 1:D:166:ASN:HA   | 1:E:517:ARG:NH1  | 2.23                     | 0.54              |
| 1:E:239:ILE:HD13 | 1:E:328:THR:HG21 | 1.90                     | 0.54              |
| 1:E:488:ASP:O    | 1:E:492:LYS:HG2  | 2.07                     | 0.54              |
| 1:E:503:GLN:HA   | 1:E:503:GLN:NE2  | 2.23                     | 0.54              |
| 1:F:26:ARG:CB    | 1:F:26:ARG:HH11  | 2.20                     | 0.54              |
| 1:H:138:ILE:O    | 1:H:142:ILE:HG12 | 2.08                     | 0.54              |
| 1:D:108:LEU:HD11 | 1:D:515:ILE:HD12 | 1.89                     | 0.54              |
| 1:E:42:THR:HG22  | 1:E:48:MET:O     | 2.08                     | 0.54              |
| 1:E:209:GLY:C    | 1:E:211:GLU:H    | 2.15                     | 0.54              |
| 1:H:206:ALA:CA   | 1:H:384:ILE:HD11 | 2.36                     | 0.54              |
| 1:E:30:LEU:O     | 1:E:34:ILE:HG13  | 2.07                     | 0.54              |
| 1:G:94:GLY:CA    | 1:G:396:LYS:HD2  | 2.38                     | 0.54              |
| 1:A:233:ARG:HH12 | 1:A:349:VAL:HG11 | 1.72                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:165:LYS:NZ   | 1:B:393:ASP:OD2  | 2.34                     | 0.54              |
| 1:E:205:LYS:O    | 1:E:377:ARG:NH1  | 2.41                     | 0.54              |
| 1:G:142:ILE:HB   | 1:G:475:LEU:CD2  | 2.36                     | 0.54              |
| 1:G:430:GLY:CA   | 1:G:434:ALA:HB2  | 2.37                     | 0.54              |
| 1:B:117:GLN:O    | 1:B:118:ASN:HB2  | 2.06                     | 0.54              |
| 1:B:222:ASP:OD1  | 1:B:360:MET:HE3  | 2.08                     | 0.54              |
| 1:B:461:GLU:HG2  | 1:B:465:LYS:HZ2  | 1.73                     | 0.54              |
| 1:D:54:ASP:OD1   | 1:D:58:ASP:HB3   | 2.06                     | 0.54              |
| 1:F:380:THR:HG22 | 1:F:383:VAL:CG2  | 2.30                     | 0.54              |
| 1:H:143:ALA:HB3  | 1:H:145:ARG:NH1  | 2.22                     | 0.54              |
| 1:D:218:GLY:HA3  | 1:D:363:VAL:O    | 2.07                     | 0.54              |
| 1:D:230:MET:HE2  | 1:D:310:ILE:O    | 2.06                     | 0.54              |
| 1:D:355:LEU:HD11 | 1:D:377:ARG:NH2  | 2.23                     | 0.54              |
| 1:D:76:HIS:HB2   | 1:E:11:ILE:HA    | 1.91                     | 0.53              |
| 1:D:134:LYS:O    | 1:D:138:ILE:HG13 | 2.08                     | 0.53              |
| 1:E:372:VAL:HG22 | 1:E:373:THR:N    | 2.23                     | 0.53              |
| 1:E:446:ILE:HG22 | 1:E:450:THR:HG23 | 1.91                     | 0.53              |
| 1:H:348:GLU:HB3  | 1:H:365:GLY:HA3  | 1.91                     | 0.53              |
| 1:C:136:GLN:HA   | 1:C:136:GLN:HE21 | 1.71                     | 0.53              |
| 1:E:258:ASN:HB3  | 1:F:258:ASN:ND2  | 2.23                     | 0.53              |
| 1:H:146:VAL:HG22 | 1:H:147:ASP:N    | 2.22                     | 0.53              |
| 1:A:33:ARG:NH1   | 1:A:109:ARG:HG3  | 2.23                     | 0.53              |
| 1:D:35:ILE:HD11  | 1:D:74:LEU:CD2   | 2.37                     | 0.53              |
| 1:E:335:ASN:HD21 | 1:E:337:LYS:HB2  | 1.74                     | 0.53              |
| 1:F:217:ARG:HA   | 1:F:372:VAL:CG2  | 2.36                     | 0.53              |
| 1:F:317:LYS:O    | 1:F:320:ASP:N    | 2.41                     | 0.53              |
| 1:G:18:ARG:HG3   | 1:G:522:ILE:HG12 | 1.90                     | 0.53              |
| 1:G:146:VAL:HG22 | 1:G:147:ASP:N    | 2.24                     | 0.53              |
| 1:H:426:ALA:HB1  | 1:H:438:GLU:HG3  | 1.91                     | 0.53              |
| 1:A:94:GLY:CA    | 1:A:396:LYS:HD2  | 2.39                     | 0.53              |
| 1:A:501:LYS:HA   | 1:A:501:LYS:HE3  | 1.88                     | 0.53              |
| 1:B:166:ASN:C    | 1:B:166:ASN:ND2  | 2.65                     | 0.53              |
| 1:B:216:VAL:O    | 1:B:372:VAL:CG2  | 2.56                     | 0.53              |
| 1:C:31:ALA:CB    | 1:C:76:HIS:CD2   | 2.91                     | 0.53              |
| 1:E:233:ARG:HH12 | 1:E:349:VAL:HG13 | 1.72                     | 0.53              |
| 1:F:12:LEU:HD23  | 1:F:13:PRO:HD2   | 1.90                     | 0.53              |
| 1:F:138:ILE:HD13 | 1:F:421:ARG:HG2  | 1.91                     | 0.53              |
| 1:G:11:ILE:CG2   | 1:G:12:LEU:H     | 2.21                     | 0.53              |
| 1:H:151:GLU:O    | 1:H:155:LEU:HD23 | 2.08                     | 0.53              |
| 1:B:82:MET:HE3   | 1:B:101:VAL:HG13 | 1.90                     | 0.53              |
| 1:D:391:LEU:O    | 1:D:395:VAL:HG23 | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:50:LYS:HD2   | 1:E:68:ILE:HD13  | 1.90                     | 0.53              |
| 1:E:146:VAL:HG22 | 1:E:147:ASP:N    | 2.21                     | 0.53              |
| 1:F:38:THR:O     | 1:F:50:LYS:CE    | 2.57                     | 0.53              |
| 1:F:147:ASP:O    | 1:F:149:ASP:N    | 2.41                     | 0.53              |
| 1:F:418:LEU:O    | 1:F:422:LEU:HB2  | 2.09                     | 0.53              |
| 1:G:409:PRO:HB2  | 1:G:489:MET:HB2  | 1.91                     | 0.53              |
| 1:A:315:ARG:HG3  | 1:A:315:ARG:NH1  | 2.24                     | 0.53              |
| 1:A:466:VAL:HG22 | 1:A:486:PRO:HG3  | 1.91                     | 0.53              |
| 1:A:473:ARG:HB2  | 1:A:477:ILE:HG13 | 1.90                     | 0.53              |
| 1:B:82:MET:CE    | 1:B:101:VAL:HG13 | 2.39                     | 0.53              |
| 1:H:232:LYS:HD2  | 1:H:352:GLU:OE2  | 2.09                     | 0.53              |
| 1:H:315:ARG:HH11 | 1:H:315:ARG:HG3  | 1.73                     | 0.53              |
| 1:C:259:ILE:HD12 | 1:C:259:ILE:N    | 2.24                     | 0.53              |
| 1:C:313:VAL:HG21 | 1:C:361:ILE:CD1  | 2.38                     | 0.53              |
| 1:C:354:LYS:HA   | 1:C:358:GLU:O    | 2.09                     | 0.53              |
| 1:D:146:VAL:HG22 | 1:D:147:ASP:N    | 2.23                     | 0.53              |
| 1:D:425:TYR:O    | 1:D:429:VAL:HG23 | 2.08                     | 0.53              |
| 1:E:460:VAL:O    | 1:E:464:VAL:HG23 | 2.07                     | 0.53              |
| 1:F:146:VAL:O    | 1:F:148:PRO:HD3  | 2.09                     | 0.53              |
| 1:G:408:LEU:HD12 | 1:G:498:LEU:HA   | 1.89                     | 0.53              |
| 1:G:417:GLU:OE2  | 1:G:470:HIS:NE2  | 2.42                     | 0.53              |
| 1:B:106:GLU:HG2  | 1:B:446:ILE:HG13 | 1.91                     | 0.53              |
| 1:E:184:GLN:NE2  | 1:E:217:ARG:NH2  | 2.57                     | 0.53              |
| 1:E:208:GLU:HB3  | 1:E:212:GLU:CG   | 2.39                     | 0.53              |
| 1:F:353:ARG:HD2  | 1:F:362:PHE:CD1  | 2.44                     | 0.53              |
| 1:H:10:VAL:HG22  | 1:H:11:ILE:N     | 2.15                     | 0.53              |
| 1:A:155:LEU:HA   | 1:A:179:VAL:HG21 | 1.91                     | 0.53              |
| 1:B:354:LYS:HA   | 1:B:358:GLU:O    | 2.08                     | 0.53              |
| 1:E:469:GLU:CB   | 1:E:477:ILE:HG21 | 2.38                     | 0.53              |
| 1:F:154:LEU:HG   | 1:F:398:VAL:HG13 | 1.89                     | 0.53              |
| 1:H:227:HIS:HB3  | 1:H:230:MET:CG   | 2.37                     | 0.53              |
| 1:A:22:ARG:CG    | 1:A:23:ASP:N     | 2.72                     | 0.52              |
| 1:B:146:VAL:HG22 | 1:B:147:ASP:N    | 2.24                     | 0.52              |
| 1:D:463:LEU:O    | 1:D:467:ILE:HG13 | 2.09                     | 0.52              |
| 1:E:353:ARG:NH2  | 1:E:364:GLU:OE2  | 2.40                     | 0.52              |
| 1:E:421:ARG:HH11 | 1:E:421:ARG:CB   | 2.09                     | 0.52              |
| 1:A:221:ILE:CD1  | 1:A:324:LEU:HD11 | 2.39                     | 0.52              |
| 1:C:217:ARG:HA   | 1:C:372:VAL:HG23 | 1.90                     | 0.52              |
| 1:G:208:GLU:HG3  | 1:G:377:ARG:HH21 | 1.74                     | 0.52              |
| 1:H:245:ALA:HB1  | 1:H:247:GLU:OE1  | 2.09                     | 0.52              |
| 1:A:227:HIS:HB3  | 1:A:230:MET:HG3  | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:388:GLU:O    | 1:B:392:GLU:HG3  | 2.08                     | 0.52              |
| 1:D:227:HIS:HB3  | 1:D:230:MET:SD   | 2.49                     | 0.52              |
| 1:E:423:ASP:O    | 1:E:426:ALA:HB3  | 2.09                     | 0.52              |
| 1:F:370:LYS:HA   | 1:F:370:LYS:CE   | 2.36                     | 0.52              |
| 1:G:410:ALA:HB3  | 1:G:494:ILE:HG22 | 1.90                     | 0.52              |
| 1:A:184:GLN:NE2  | 1:A:184:GLN:HA   | 2.24                     | 0.52              |
| 1:A:465:LYS:O    | 1:A:468:SER:HB3  | 2.09                     | 0.52              |
| 1:B:22:ARG:CG    | 1:B:23:ASP:N     | 2.71                     | 0.52              |
| 1:B:425:TYR:O    | 1:B:429:VAL:HG23 | 2.10                     | 0.52              |
| 1:C:388:GLU:O    | 1:C:392:GLU:HG3  | 2.09                     | 0.52              |
| 1:D:286:THR:HG21 | 1:D:339:LEU:HG   | 1.92                     | 0.52              |
| 1:E:290:VAL:HG22 | 1:E:311:MET:HE2  | 1.91                     | 0.52              |
| 1:F:205:LYS:O    | 1:F:377:ARG:NH1  | 2.42                     | 0.52              |
| 1:H:372:VAL:HG22 | 1:H:373:THR:H    | 1.74                     | 0.52              |
| 1:A:217:ARG:HA   | 1:A:372:VAL:HG23 | 1.92                     | 0.52              |
| 1:B:25:GLN:O     | 1:B:29:ILE:HG13  | 2.10                     | 0.52              |
| 1:B:315:ARG:HG3  | 1:B:315:ARG:NH1  | 2.16                     | 0.52              |
| 1:C:506:LYS:O    | 1:C:510:GLU:CG   | 2.57                     | 0.52              |
| 1:D:31:ALA:CB    | 1:D:76:HIS:CD2   | 2.93                     | 0.52              |
| 1:H:38:THR:O     | 1:H:50:LYS:CE    | 2.57                     | 0.52              |
| 1:A:195:VAL:HB   | 1:A:399:LYS:HG3  | 1.89                     | 0.52              |
| 1:C:335:ASN:OD1  | 1:C:337:LYS:HB2  | 2.09                     | 0.52              |
| 1:D:293:VAL:HG21 | 1:D:297:ILE:HD11 | 1.92                     | 0.52              |
| 1:D:342:GLU:OE2  | 1:D:342:GLU:N    | 2.40                     | 0.52              |
| 1:E:286:THR:HA   | 1:E:341:PRO:HG3  | 1.91                     | 0.52              |
| 1:G:462:MET:O    | 1:G:466:VAL:HG23 | 2.10                     | 0.52              |
| 1:H:76:HIS:CD2   | 1:H:78:ALA:H     | 2.28                     | 0.52              |
| 1:H:170:HIS:CE1  | 1:H:210:VAL:HB   | 2.44                     | 0.52              |
| 1:H:460:VAL:O    | 1:H:464:VAL:HG23 | 2.09                     | 0.52              |
| 1:B:496:GLU:OE1  | 1:B:501:LYS:NZ   | 2.31                     | 0.52              |
| 1:C:368:ASN:ND2  | 1:C:370:LYS:HE3  | 2.24                     | 0.52              |
| 1:C:394:ALA:O    | 1:C:398:VAL:HG23 | 2.09                     | 0.52              |
| 1:E:22:ARG:CG    | 1:E:23:ASP:N     | 2.72                     | 0.52              |
| 1:E:233:ARG:NH1  | 1:E:349:VAL:HG13 | 2.24                     | 0.52              |
| 1:E:260:THR:H    | 1:E:264:GLN:HE21 | 1.56                     | 0.52              |
| 1:F:380:THR:CG2  | 1:F:383:VAL:H    | 2.20                     | 0.52              |
| 1:A:193:TYR:CE2  | 1:A:402:MET:HE2  | 2.45                     | 0.52              |
| 1:D:147:ASP:O    | 1:D:149:ASP:N    | 2.43                     | 0.52              |
| 1:E:31:ALA:HA    | 1:E:34:ILE:HD12  | 1.91                     | 0.52              |
| 1:G:227:HIS:HE2  | 1:H:334:THR:HB   | 1.75                     | 0.52              |
| 1:G:524:ALA:O    | 1:G:525:LYS:HD2  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:182:VAL:HG22 | 1:A:395:VAL:HG13 | 1.92                     | 0.52              |
| 1:A:461:GLU:HG2  | 1:A:465:LYS:NZ   | 2.25                     | 0.52              |
| 1:C:13:PRO:O     | 1:C:16:THR:HB    | 2.10                     | 0.52              |
| 1:D:424:GLU:O    | 1:D:428:GLN:HG2  | 2.10                     | 0.52              |
| 1:F:29:ILE:HG23  | 1:F:108:LEU:HB3  | 1.92                     | 0.52              |
| 1:G:380:THR:CG2  | 1:G:383:VAL:H    | 2.19                     | 0.52              |
| 1:A:423:ASP:OD1  | 1:A:427:LYS:HE2  | 2.10                     | 0.52              |
| 1:B:22:ARG:HG3   | 1:B:23:ASP:N     | 2.24                     | 0.52              |
| 1:B:383:VAL:O    | 1:B:387:VAL:HG23 | 2.09                     | 0.52              |
| 1:C:126:LYS:NZ   | 1:C:126:LYS:HB3  | 2.25                     | 0.52              |
| 1:F:151:GLU:O    | 1:F:155:LEU:HD23 | 2.10                     | 0.52              |
| 1:G:45:PRO:HA    | 1:G:164:GLY:HA2  | 1.92                     | 0.52              |
| 1:H:483:GLU:OE1  | 1:H:483:GLU:HA   | 2.09                     | 0.52              |
| 1:D:59:ILE:HD12  | 1:D:59:ILE:N     | 2.25                     | 0.51              |
| 1:E:11:ILE:C     | 1:E:11:ILE:CD1   | 2.80                     | 0.51              |
| 1:E:330:ALA:HB2  | 1:E:345:GLY:HA3  | 1.92                     | 0.51              |
| 1:E:470:HIS:CE1  | 1:E:475:LEU:HA   | 2.45                     | 0.51              |
| 1:H:17:GLN:NE2   | 1:H:17:GLN:H     | 2.07                     | 0.51              |
| 1:H:92:GLU:O     | 1:H:499:ARG:HD3  | 2.11                     | 0.51              |
| 1:H:217:ARG:HB3  | 1:H:217:ARG:HH11 | 1.75                     | 0.51              |
| 1:H:293:VAL:HG21 | 1:H:297:ILE:HD11 | 1.92                     | 0.51              |
| 1:B:184:GLN:HE22 | 1:B:217:ARG:HH21 | 1.54                     | 0.51              |
| 1:C:217:ARG:HB3  | 1:C:217:ARG:HH11 | 1.75                     | 0.51              |
| 1:D:370:LYS:HE2  | 1:D:370:LYS:CA   | 2.39                     | 0.51              |
| 1:E:327:ALA:O    | 1:E:366:CYS:HB3  | 2.10                     | 0.51              |
| 1:A:73:ASP:O     | 1:B:13:PRO:HD3   | 2.10                     | 0.51              |
| 1:A:106:GLU:HG2  | 1:A:446:ILE:CG1  | 2.40                     | 0.51              |
| 1:A:445:LYS:O    | 1:A:448:PRO:HD2  | 2.10                     | 0.51              |
| 1:B:257:ILE:HG22 | 1:B:259:ILE:HD12 | 1.93                     | 0.51              |
| 1:D:94:GLY:HA2   | 1:D:396:LYS:HD2  | 1.91                     | 0.51              |
| 1:E:59:ILE:HD12  | 1:E:59:ILE:H     | 1.73                     | 0.51              |
| 1:F:126:LYS:HB3  | 1:F:126:LYS:HZ2  | 1.74                     | 0.51              |
| 1:F:201:LYS:HB2  | 1:F:323:LYS:HE3  | 1.92                     | 0.51              |
| 1:A:170:HIS:HD2  | 1:A:211:GLU:OE1  | 1.93                     | 0.51              |
| 1:B:154:LEU:HG   | 1:B:398:VAL:HG13 | 1.92                     | 0.51              |
| 1:D:142:ILE:HB   | 1:D:475:LEU:CD2  | 2.41                     | 0.51              |
| 1:E:33:ARG:NH1   | 1:E:109:ARG:HG3  | 2.26                     | 0.51              |
| 1:E:94:GLY:HA2   | 1:E:396:LYS:HD2  | 1.93                     | 0.51              |
| 1:E:147:ASP:O    | 1:E:149:ASP:N    | 2.43                     | 0.51              |
| 1:G:184:GLN:NE2  | 1:G:217:ARG:NH2  | 2.59                     | 0.51              |
| 1:G:250:LYS:NZ   | 1:H:253:THR:HA   | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:253:THR:O    | 1:H:254:ASP:C    | 2.54                     | 0.51              |
| 1:A:483:GLU:HG3  | 1:A:485:LYS:HZ1  | 1.74                     | 0.51              |
| 1:E:417:GLU:OE1  | 1:E:421:ARG:NH1  | 2.43                     | 0.51              |
| 1:H:136:GLN:HA   | 1:H:136:GLN:HE21 | 1.75                     | 0.51              |
| 1:H:335:ASN:OD1  | 1:H:337:LYS:HB2  | 2.11                     | 0.51              |
| 1:F:449:LYS:HE3  | 1:F:459:THR:CG2  | 2.40                     | 0.51              |
| 1:H:239:ILE:HD11 | 1:H:347:ALA:CB   | 2.39                     | 0.51              |
| 1:H:465:LYS:O    | 1:H:468:SER:HB3  | 2.09                     | 0.51              |
| 1:A:82:MET:HE1   | 1:A:104:ALA:CB   | 2.41                     | 0.51              |
| 1:A:460:VAL:O    | 1:A:464:VAL:HG23 | 2.11                     | 0.51              |
| 1:B:217:ARG:HA   | 1:B:372:VAL:HG23 | 1.92                     | 0.51              |
| 1:B:409:PRO:HB3  | 1:B:490:LEU:HD13 | 1.93                     | 0.51              |
| 1:C:370:LYS:HE2  | 1:C:370:LYS:CA   | 2.41                     | 0.51              |
| 1:C:392:GLU:O    | 1:C:396:LYS:HE3  | 2.11                     | 0.51              |
| 1:D:188:LYS:HD3  | 1:D:193:TYR:CE1  | 2.45                     | 0.51              |
| 1:E:446:ILE:HD12 | 1:E:446:ILE:H    | 1.76                     | 0.51              |
| 1:G:136:GLN:HA   | 1:G:136:GLN:NE2  | 2.26                     | 0.51              |
| 1:G:210:VAL:HA   | 1:G:377:ARG:O    | 2.11                     | 0.51              |
| 1:G:313:VAL:HG21 | 1:G:361:ILE:HD13 | 1.92                     | 0.51              |
| 1:H:429:VAL:HG21 | 1:H:437:ILE:CD1  | 2.41                     | 0.51              |
| 1:B:348:GLU:CB   | 1:B:365:GLY:HA3  | 2.40                     | 0.51              |
| 1:B:372:VAL:HG22 | 1:B:373:THR:N    | 2.26                     | 0.51              |
| 1:C:22:ARG:CG    | 1:C:23:ASP:N     | 2.74                     | 0.51              |
| 1:C:145:ARG:HG2  | 1:C:145:ARG:HH11 | 1.76                     | 0.51              |
| 1:C:293:VAL:HG21 | 1:C:297:ILE:HD11 | 1.92                     | 0.51              |
| 1:H:138:ILE:HD13 | 1:H:421:ARG:HG2  | 1.92                     | 0.51              |
| 1:B:196:ASP:OD1  | 1:B:198:ASP:HB2  | 2.11                     | 0.51              |
| 1:D:397:VAL:O    | 1:D:401:VAL:HG23 | 2.11                     | 0.51              |
| 1:G:355:LEU:O    | 1:G:356:ALA:HB3  | 2.11                     | 0.51              |
| 1:H:515:ILE:C    | 1:H:517:ARG:H    | 2.19                     | 0.51              |
| 1:B:258:ASN:HB3  | 1:C:258:ASN:ND2  | 2.26                     | 0.51              |
| 1:C:430:GLY:CA   | 1:C:434:ALA:HB2  | 2.41                     | 0.51              |
| 1:D:292:PHE:CD1  | 1:D:324:LEU:HD13 | 2.45                     | 0.51              |
| 1:E:51:MET:CE    | 1:F:77:PRO:HB2   | 2.41                     | 0.51              |
| 1:G:59:ILE:HD12  | 1:G:59:ILE:H     | 1.76                     | 0.51              |
| 1:A:146:VAL:HG22 | 1:A:147:ASP:H    | 1.75                     | 0.50              |
| 1:A:170:HIS:HD2  | 1:A:211:GLU:CD   | 2.19                     | 0.50              |
| 1:B:412:GLY:HA2  | 1:B:415:GLU:CG   | 2.41                     | 0.50              |
| 1:D:498:LEU:O    | 1:D:498:LEU:HD22 | 2.11                     | 0.50              |
| 1:F:266:MET:O    | 1:F:270:GLU:HG3  | 2.11                     | 0.50              |
| 1:F:498:LEU:O    | 1:F:498:LEU:HD22 | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:269:LEU:HD12 | 1:C:251:THR:HG23 | 1.91                     | 0.50              |
| 1:C:215:LEU:HD11 | 1:C:372:VAL:CG2  | 2.40                     | 0.50              |
| 1:D:72:ILE:HG22  | 1:D:73:ASP:N     | 2.26                     | 0.50              |
| 1:E:445:LYS:O    | 1:E:448:PRO:HD2  | 2.11                     | 0.50              |
| 1:F:297:ILE:HD12 | 1:F:314:ARG:HB3  | 1.92                     | 0.50              |
| 1:G:216:VAL:O    | 1:G:218:GLY:N    | 2.43                     | 0.50              |
| 1:G:259:ILE:HG23 | 1:G:264:GLN:HB2  | 1.93                     | 0.50              |
| 1:C:126:LYS:O    | 1:C:130:LEU:HG   | 2.11                     | 0.50              |
| 1:D:155:LEU:HD22 | 1:D:179:VAL:HG21 | 1.93                     | 0.50              |
| 1:D:271:GLN:O    | 1:D:275:MET:HG3  | 2.10                     | 0.50              |
| 1:E:54:ASP:OD1   | 1:E:58:ASP:HB3   | 2.11                     | 0.50              |
| 1:G:188:LYS:HD3  | 1:G:193:TYR:CE1  | 2.46                     | 0.50              |
| 1:A:77:PRO:CG    | 1:H:53:VAL:HG21  | 2.41                     | 0.50              |
| 1:B:233:ARG:HH11 | 1:B:233:ARG:HG3  | 1.77                     | 0.50              |
| 1:B:461:GLU:HG2  | 1:B:465:LYS:NZ   | 2.25                     | 0.50              |
| 1:C:51:MET:HE3   | 1:D:77:PRO:HB2   | 1.94                     | 0.50              |
| 1:C:227:HIS:HD1  | 1:C:229:ARG:H    | 1.58                     | 0.50              |
| 1:D:230:MET:HE1  | 1:D:312:ALA:CB   | 2.39                     | 0.50              |
| 1:E:106:GLU:HG2  | 1:E:446:ILE:HG13 | 1.93                     | 0.50              |
| 1:E:204:LYS:HB3  | 1:E:384:ILE:CG2  | 2.40                     | 0.50              |
| 1:E:315:ARG:HH11 | 1:E:315:ARG:HG3  | 1.76                     | 0.50              |
| 1:F:116:ASP:C    | 1:F:118:ASN:H    | 2.19                     | 0.50              |
| 1:F:117:GLN:O    | 1:F:118:ASN:HB2  | 2.10                     | 0.50              |
| 1:G:17:GLN:NE2   | 1:G:17:GLN:N     | 2.57                     | 0.50              |
| 1:G:117:GLN:O    | 1:G:118:ASN:HB2  | 2.10                     | 0.50              |
| 1:A:271:GLN:O    | 1:A:275:MET:HG3  | 2.11                     | 0.50              |
| 1:A:418:LEU:O    | 1:A:422:LEU:HB2  | 2.12                     | 0.50              |
| 1:C:215:LEU:HD11 | 1:C:372:VAL:HG21 | 1.93                     | 0.50              |
| 1:D:421:ARG:HB2  | 1:D:421:ARG:NH1  | 2.20                     | 0.50              |
| 1:E:82:MET:CE    | 1:E:101:VAL:HG13 | 2.42                     | 0.50              |
| 1:E:221:ILE:CD1  | 1:E:324:LEU:HD11 | 2.41                     | 0.50              |
| 1:G:239:ILE:H    | 1:G:239:ILE:HD12 | 1.75                     | 0.50              |
| 1:H:415:GLU:HG3  | 1:H:447:ILE:HB   | 1.94                     | 0.50              |
| 1:A:182:VAL:CG2  | 1:A:395:VAL:HG13 | 2.42                     | 0.50              |
| 1:D:51:MET:HB2   | 1:E:518:ILE:HD13 | 1.94                     | 0.50              |
| 1:D:258:ASN:CB   | 1:E:258:ASN:HD21 | 2.14                     | 0.50              |
| 1:D:450:THR:O    | 1:D:454:ASN:ND2  | 2.44                     | 0.50              |
| 1:E:462:MET:HE3  | 1:E:465:LYS:HD2  | 1.94                     | 0.50              |
| 1:H:166:ASN:C    | 1:H:166:ASN:HD22 | 2.20                     | 0.50              |
| 1:A:147:ASP:O    | 1:A:149:ASP:N    | 2.45                     | 0.50              |
| 1:B:146:VAL:HG22 | 1:B:147:ASP:H    | 1.77                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:256:LYS:HE3  | 1:D:254:ASP:OD1  | 2.11                     | 0.50              |
| 1:D:303:HIS:NE2  | 1:E:335:ASN:HB3  | 2.26                     | 0.50              |
| 1:E:35:ILE:HD11  | 1:E:74:LEU:CD2   | 2.42                     | 0.50              |
| 1:E:92:GLU:O     | 1:E:499:ARG:HD3  | 2.12                     | 0.50              |
| 1:G:138:ILE:O    | 1:G:142:ILE:HG23 | 2.12                     | 0.50              |
| 1:G:175:ALA:O    | 1:G:179:VAL:HG23 | 2.11                     | 0.50              |
| 1:H:29:ILE:O     | 1:H:33:ARG:HG3   | 2.11                     | 0.50              |
| 1:A:218:GLY:HA3  | 1:A:363:VAL:O    | 2.12                     | 0.50              |
| 1:B:125:ILE:HD13 | 1:B:517:ARG:HG2  | 1.93                     | 0.50              |
| 1:C:134:LYS:O    | 1:C:138:ILE:HG13 | 2.12                     | 0.50              |
| 1:D:89:GLN:OE1   | 1:D:503:GLN:HG3  | 2.11                     | 0.50              |
| 1:D:462:MET:O    | 1:D:466:VAL:HG23 | 2.12                     | 0.50              |
| 1:E:277:LYS:HB2  | 1:E:304:TYR:CE2  | 2.47                     | 0.50              |
| 1:G:10:VAL:CG1   | 1:G:11:ILE:H     | 2.13                     | 0.50              |
| 1:G:215:LEU:HD11 | 1:G:372:VAL:HG21 | 1.94                     | 0.50              |
| 1:H:138:ILE:CD1  | 1:H:421:ARG:HG2  | 2.42                     | 0.50              |
| 1:H:286:THR:HG21 | 1:H:339:LEU:HG   | 1.93                     | 0.50              |
| 1:A:458:ASP:C    | 1:A:458:ASP:OD2  | 2.55                     | 0.50              |
| 1:E:126:LYS:NZ   | 1:E:126:LYS:HB3  | 2.27                     | 0.50              |
| 1:E:167:ALA:O    | 1:E:169:SER:N    | 2.45                     | 0.50              |
| 1:E:209:GLY:C    | 1:E:211:GLU:N    | 2.69                     | 0.50              |
| 1:G:408:LEU:O    | 1:G:495:ILE:HB   | 2.12                     | 0.50              |
| 1:A:91:LYS:HB2   | 1:A:91:LYS:HZ2   | 1.77                     | 0.49              |
| 1:B:48:MET:HE2   | 1:B:48:MET:HA    | 1.95                     | 0.49              |
| 1:B:175:ALA:O    | 1:B:179:VAL:HG23 | 2.12                     | 0.49              |
| 1:B:225:VAL:HG23 | 1:B:352:GLU:OE1  | 2.12                     | 0.49              |
| 1:C:217:ARG:HB3  | 1:C:217:ARG:NH1  | 2.27                     | 0.49              |
| 1:E:106:GLU:HG2  | 1:E:446:ILE:HG12 | 1.93                     | 0.49              |
| 1:E:462:MET:CE   | 1:E:486:PRO:HD3  | 2.42                     | 0.49              |
| 1:H:244:GLU:OE1  | 1:H:336:VAL:HG22 | 2.12                     | 0.49              |
| 1:A:150:ASP:OD1  | 1:A:153:THR:HG23 | 2.12                     | 0.49              |
| 1:A:513:ILE:O    | 1:A:517:ARG:HG3  | 2.12                     | 0.49              |
| 1:B:120:HIS:CG   | 1:B:121:PRO:HD2  | 2.48                     | 0.49              |
| 1:B:259:ILE:HD12 | 1:B:259:ILE:N    | 2.27                     | 0.49              |
| 1:C:72:ILE:HG22  | 1:C:74:LEU:HD23  | 1.92                     | 0.49              |
| 1:C:188:LYS:HD3  | 1:C:193:TYR:CE1  | 2.46                     | 0.49              |
| 1:C:498:LEU:HD13 | 1:C:502:LYS:HD3  | 1.95                     | 0.49              |
| 1:D:82:MET:HE1   | 1:D:104:ALA:HB3  | 1.94                     | 0.49              |
| 1:D:209:GLY:C    | 1:D:211:GLU:N    | 2.70                     | 0.49              |
| 1:D:393:ASP:O    | 1:D:397:VAL:HG22 | 2.12                     | 0.49              |
| 1:E:11:ILE:HG23  | 1:E:12:LEU:H     | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:110:LYS:HE3  | 1:E:442:ASP:OD1  | 2.11                     | 0.49              |
| 1:E:394:ALA:O    | 1:E:397:VAL:HG22 | 2.12                     | 0.49              |
| 1:F:72:ILE:HG22  | 1:F:74:LEU:HD23  | 1.95                     | 0.49              |
| 1:A:123:ILE:HG21 | 1:A:432:LYS:HB2  | 1.95                     | 0.49              |
| 1:A:227:HIS:ND1  | 1:A:228:PRO:HD2  | 2.28                     | 0.49              |
| 1:E:247:GLU:HA   | 1:E:276:LEU:HD11 | 1.94                     | 0.49              |
| 1:F:476:GLY:HA3  | 1:F:490:LEU:HD22 | 1.93                     | 0.49              |
| 1:H:239:ILE:HD11 | 1:H:347:ALA:HB3  | 1.93                     | 0.49              |
| 1:H:241:LEU:CD2  | 1:H:330:ALA:HB3  | 2.42                     | 0.49              |
| 1:H:245:ALA:HB1  | 1:H:247:GLU:HG2  | 1.95                     | 0.49              |
| 1:A:188:LYS:HB2  | 1:A:193:TYR:HA   | 1.94                     | 0.49              |
| 1:A:209:GLY:O    | 1:A:211:GLU:N    | 2.45                     | 0.49              |
| 1:A:251:THR:HG23 | 1:H:269:LEU:CD1  | 2.40                     | 0.49              |
| 1:C:35:ILE:HD12  | 1:C:69:LEU:CD2   | 2.43                     | 0.49              |
| 1:C:125:ILE:CD1  | 1:C:517:ARG:HG2  | 2.41                     | 0.49              |
| 1:C:432:LYS:O    | 1:C:435:LEU:HB2  | 2.11                     | 0.49              |
| 1:E:99:THR:HG23  | 1:E:447:ILE:HD12 | 1.95                     | 0.49              |
| 1:F:216:VAL:O    | 1:F:218:GLY:N    | 2.45                     | 0.49              |
| 1:F:462:MET:CE   | 1:F:465:LYS:HD2  | 2.42                     | 0.49              |
| 1:C:138:ILE:O    | 1:C:142:ILE:HG23 | 2.12                     | 0.49              |
| 1:C:293:VAL:CG2  | 1:C:297:ILE:HD11 | 2.42                     | 0.49              |
| 1:C:304:TYR:O    | 1:C:308:TYR:HD1  | 1.96                     | 0.49              |
| 1:D:12:LEU:HD23  | 1:D:13:PRO:HD2   | 1.93                     | 0.49              |
| 1:D:409:PRO:HA   | 1:D:495:ILE:HG22 | 1.93                     | 0.49              |
| 1:G:506:LYS:O    | 1:G:510:GLU:CG   | 2.60                     | 0.49              |
| 1:H:146:VAL:HG22 | 1:H:147:ASP:H    | 1.76                     | 0.49              |
| 1:A:205:LYS:HE3  | 1:A:360:MET:SD   | 2.52                     | 0.49              |
| 1:D:136:GLN:HA   | 1:D:136:GLN:HE21 | 1.78                     | 0.49              |
| 1:D:445:LYS:C    | 1:D:448:PRO:HD2  | 2.37                     | 0.49              |
| 1:E:72:ILE:HD11  | 1:F:522:ILE:CD1  | 2.37                     | 0.49              |
| 1:E:413:ALA:N    | 1:E:414:PRO:CD   | 2.76                     | 0.49              |
| 1:A:103:ILE:O    | 1:A:107:LEU:HB2  | 2.12                     | 0.49              |
| 1:A:208:GLU:HB3  | 1:A:212:GLU:CG   | 2.42                     | 0.49              |
| 1:C:146:VAL:HG22 | 1:C:147:ASP:H    | 1.78                     | 0.49              |
| 1:E:170:HIS:HD2  | 1:E:211:GLU:OE1  | 1.96                     | 0.49              |
| 1:F:38:THR:O     | 1:F:50:LYS:HE3   | 2.12                     | 0.49              |
| 1:C:17:GLN:H     | 1:C:17:GLN:CD    | 2.21                     | 0.49              |
| 1:C:197:LEU:HD22 | 1:C:395:VAL:CG1  | 2.42                     | 0.49              |
| 1:C:369:PRO:HB2  | 1:C:371:ALA:O    | 2.13                     | 0.49              |
| 1:D:136:GLN:HA   | 1:D:136:GLN:NE2  | 2.27                     | 0.49              |
| 1:D:210:VAL:O    | 1:D:210:VAL:HG12 | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:248:VAL:HG11 | 1:E:272:GLU:OE2  | 2.12                     | 0.49              |
| 1:E:400:ASP:OD1  | 1:E:499:ARG:HD2  | 2.12                     | 0.49              |
| 1:E:458:ASP:OD2  | 1:E:458:ASP:C    | 2.56                     | 0.49              |
| 1:G:126:LYS:HB3  | 1:G:126:LYS:HZ2  | 1.77                     | 0.49              |
| 1:G:458:ASP:OD1  | 1:G:461:GLU:HB2  | 2.13                     | 0.49              |
| 1:H:242:ILE:HD11 | 1:H:339:LEU:HD22 | 1.94                     | 0.49              |
| 1:A:123:ILE:HG21 | 1:A:432:LYS:CB   | 2.43                     | 0.49              |
| 1:A:272:GLU:HA   | 1:A:275:MET:CE   | 2.43                     | 0.49              |
| 1:B:73:ASP:O     | 1:C:13:PRO:HD3   | 2.12                     | 0.49              |
| 1:B:81:MET:CE    | 1:B:514:MET:SD   | 2.98                     | 0.49              |
| 1:C:179:VAL:O    | 1:C:183:LYS:HG3  | 2.13                     | 0.49              |
| 1:D:18:ARG:HG3   | 1:D:522:ILE:HG12 | 1.95                     | 0.49              |
| 1:E:13:PRO:O     | 1:E:16:THR:HB    | 2.13                     | 0.49              |
| 1:F:156:LYS:O    | 1:F:157:ILE:C    | 2.56                     | 0.49              |
| 1:F:204:LYS:HD2  | 1:F:384:ILE:CG2  | 2.43                     | 0.49              |
| 1:F:211:GLU:HA   | 1:F:211:GLU:OE1  | 2.13                     | 0.49              |
| 1:G:123:ILE:HG21 | 1:G:432:LYS:CB   | 2.36                     | 0.49              |
| 1:H:154:LEU:HG   | 1:H:398:VAL:HG13 | 1.93                     | 0.49              |
| 1:A:227:HIS:HD1  | 1:A:229:ARG:H    | 1.61                     | 0.49              |
| 1:E:75:GLN:HG3   | 1:F:12:LEU:C     | 2.38                     | 0.49              |
| 1:E:477:ILE:HD13 | 1:E:488:ASP:HA   | 1.94                     | 0.49              |
| 1:F:311:MET:HE1  | 1:F:350:VAL:CG1  | 2.40                     | 0.49              |
| 1:G:69:LEU:HB3   | 1:G:83:VAL:HG22  | 1.95                     | 0.49              |
| 1:G:182:VAL:HG13 | 1:G:195:VAL:HG11 | 1.94                     | 0.49              |
| 1:H:342:GLU:H    | 1:H:342:GLU:CD   | 2.21                     | 0.49              |
| 1:A:144:ILE:CD1  | 1:A:490:LEU:HD21 | 2.40                     | 0.48              |
| 1:C:48:MET:HE2   | 1:C:48:MET:HA    | 1.94                     | 0.48              |
| 1:C:99:THR:O     | 1:C:103:ILE:HG13 | 2.12                     | 0.48              |
| 1:C:430:GLY:HA2  | 1:C:434:ALA:HB2  | 1.94                     | 0.48              |
| 1:D:182:VAL:CG2  | 1:D:395:VAL:HG13 | 2.43                     | 0.48              |
| 1:D:503:GLN:HA   | 1:D:503:GLN:NE2  | 2.28                     | 0.48              |
| 1:E:109:ARG:HG2  | 1:E:109:ARG:NH1  | 2.24                     | 0.48              |
| 1:E:145:ARG:HG2  | 1:E:145:ARG:NH1  | 2.28                     | 0.48              |
| 1:F:333:VAL:HG21 | 1:F:339:LEU:HD13 | 1.95                     | 0.48              |
| 1:G:304:TYR:O    | 1:G:308:TYR:HD1  | 1.95                     | 0.48              |
| 1:H:404:ASP:OD1  | 1:H:499:ARG:HB2  | 2.13                     | 0.48              |
| 1:B:143:ALA:HB3  | 1:B:145:ARG:NH1  | 2.28                     | 0.48              |
| 1:B:215:LEU:HD11 | 1:B:372:VAL:HG21 | 1.96                     | 0.48              |
| 1:C:348:GLU:O    | 1:C:349:VAL:CG2  | 2.59                     | 0.48              |
| 1:D:221:ILE:CD1  | 1:D:324:LEU:HD11 | 2.43                     | 0.48              |
| 1:E:433:GLU:H    | 1:E:433:GLU:CD   | 2.21                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:54:ASP:OD1   | 1:G:58:ASP:CB    | 2.54                     | 0.48              |
| 1:B:52:LEU:HD11  | 1:B:68:ILE:HA    | 1.95                     | 0.48              |
| 1:B:314:ARG:HD2  | 1:B:315:ARG:HD3  | 1.96                     | 0.48              |
| 1:B:423:ASP:OD1  | 1:B:427:LYS:HE2  | 2.12                     | 0.48              |
| 1:B:458:ASP:OD2  | 1:B:458:ASP:C    | 2.55                     | 0.48              |
| 1:C:75:GLN:CG    | 1:D:10:VAL:HG13  | 2.42                     | 0.48              |
| 1:C:154:LEU:CD2  | 1:C:402:MET:HE3  | 2.43                     | 0.48              |
| 1:A:49:ASP:OD1   | 1:A:63:ASN:HB2   | 2.13                     | 0.48              |
| 1:A:94:GLY:HA3   | 1:A:396:LYS:HD2  | 1.94                     | 0.48              |
| 1:A:146:VAL:HG22 | 1:A:147:ASP:N    | 2.29                     | 0.48              |
| 1:A:197:LEU:HD22 | 1:A:395:VAL:HG12 | 1.96                     | 0.48              |
| 1:A:235:GLU:O    | 1:A:236:ASN:O    | 2.32                     | 0.48              |
| 1:B:458:ASP:O    | 1:B:459:THR:C    | 2.57                     | 0.48              |
| 1:D:123:ILE:HG21 | 1:D:432:LYS:HB3  | 1.91                     | 0.48              |
| 1:D:487:ALA:HB3  | 1:D:489:MET:CE   | 2.42                     | 0.48              |
| 1:E:75:GLN:HE21  | 1:F:13:PRO:HA    | 1.79                     | 0.48              |
| 1:E:204:LYS:HD2  | 1:E:384:ILE:HG22 | 1.94                     | 0.48              |
| 1:E:232:LYS:HD2  | 1:E:352:GLU:OE2  | 2.13                     | 0.48              |
| 1:E:257:ILE:HG22 | 1:E:259:ILE:CD1  | 2.41                     | 0.48              |
| 1:F:23:ASP:O     | 1:F:27:LEU:HG    | 2.14                     | 0.48              |
| 1:G:450:THR:O    | 1:G:454:ASN:ND2  | 2.46                     | 0.48              |
| 1:G:501:LYS:HA   | 1:G:501:LYS:HE3  | 1.95                     | 0.48              |
| 1:A:397:VAL:HA   | 1:A:400:ASP:OD2  | 2.14                     | 0.48              |
| 1:B:489:MET:HE2  | 1:B:489:MET:HA   | 1.95                     | 0.48              |
| 1:C:166:ASN:O    | 1:C:168:GLU:HG2  | 2.14                     | 0.48              |
| 1:C:342:GLU:OE2  | 1:C:342:GLU:N    | 2.46                     | 0.48              |
| 1:D:63:ASN:O     | 1:D:63:ASN:ND2   | 2.47                     | 0.48              |
| 1:E:167:ALA:C    | 1:E:169:SER:N    | 2.71                     | 0.48              |
| 1:C:330:ALA:HB2  | 1:C:345:GLY:HA3  | 1.94                     | 0.48              |
| 1:C:370:LYS:HA   | 1:C:370:LYS:CE   | 2.43                     | 0.48              |
| 1:F:81:MET:HE1   | 1:F:515:ILE:HG12 | 1.96                     | 0.48              |
| 1:G:119:ILE:HD11 | 1:G:435:LEU:HD23 | 1.95                     | 0.48              |
| 1:G:219:VAL:HG12 | 1:G:220:VAL:N    | 2.29                     | 0.48              |
| 1:A:143:ALA:HB3  | 1:A:145:ARG:HH12 | 1.79                     | 0.48              |
| 1:A:409:PRO:HA   | 1:A:495:ILE:HG22 | 1.94                     | 0.48              |
| 1:B:35:ILE:HG21  | 1:B:82:MET:CB    | 2.44                     | 0.48              |
| 1:B:100:ALA:O    | 1:B:508:ALA:HB2  | 2.14                     | 0.48              |
| 1:B:450:THR:O    | 1:B:454:ASN:ND2  | 2.47                     | 0.48              |
| 1:C:243:ASN:OD1  | 1:C:295:LYS:HE3  | 2.14                     | 0.48              |
| 1:E:304:TYR:O    | 1:E:308:TYR:HD1  | 1.97                     | 0.48              |
| 1:E:475:LEU:HD12 | 1:E:475:LEU:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:315:ARG:HG3  | 1:F:315:ARG:NH1  | 2.22                     | 0.48              |
| 1:F:369:PRO:O    | 1:F:370:LYS:HE2  | 2.13                     | 0.48              |
| 1:G:273:GLU:HG2  | 1:G:300:LEU:CD1  | 2.43                     | 0.48              |
| 1:H:458:ASP:OD2  | 1:H:458:ASP:C    | 2.56                     | 0.48              |
| 1:A:297:ILE:HG22 | 1:A:302:GLN:HG3  | 1.96                     | 0.48              |
| 1:B:143:ALA:HB3  | 1:B:145:ARG:HH12 | 1.79                     | 0.48              |
| 1:B:212:GLU:HB2  | 1:B:377:ARG:HG3  | 1.96                     | 0.48              |
| 1:B:524:ALA:O    | 1:B:525:LYS:HD2  | 2.12                     | 0.48              |
| 1:C:120:HIS:ND1  | 1:C:122:SER:CB   | 2.76                     | 0.48              |
| 1:C:423:ASP:O    | 1:C:426:ALA:HB3  | 2.13                     | 0.48              |
| 1:D:158:ALA:O    | 1:D:162:ILE:HG13 | 2.13                     | 0.48              |
| 1:E:22:ARG:HG3   | 1:E:23:ASP:N     | 2.29                     | 0.48              |
| 1:E:158:ALA:O    | 1:E:162:ILE:HG13 | 2.12                     | 0.48              |
| 1:E:280:VAL:HG11 | 1:E:304:TYR:HB3  | 1.96                     | 0.48              |
| 1:E:317:LYS:O    | 1:E:320:ASP:N    | 2.47                     | 0.48              |
| 1:H:50:LYS:HD2   | 1:H:68:ILE:HD13  | 1.96                     | 0.48              |
| 1:B:269:LEU:HD12 | 1:C:251:THR:CG2  | 2.44                     | 0.48              |
| 1:E:432:LYS:O    | 1:E:435:LEU:HB2  | 2.13                     | 0.48              |
| 1:F:226:VAL:O    | 1:F:226:VAL:HG22 | 2.14                     | 0.48              |
| 1:F:241:LEU:HD22 | 1:F:330:ALA:HB3  | 1.95                     | 0.48              |
| 1:G:16:THR:HG23  | 1:G:523:ALA:O    | 2.14                     | 0.48              |
| 1:G:146:VAL:HG22 | 1:G:147:ASP:H    | 1.79                     | 0.48              |
| 1:H:99:THR:O     | 1:H:103:ILE:HG13 | 2.13                     | 0.48              |
| 1:B:116:ASP:C    | 1:B:118:ASN:H    | 2.22                     | 0.48              |
| 1:C:524:ALA:O    | 1:C:525:LYS:HE2  | 2.14                     | 0.48              |
| 1:D:156:LYS:O    | 1:D:157:ILE:C    | 2.56                     | 0.48              |
| 1:D:509:SER:O    | 1:D:513:ILE:HG13 | 2.13                     | 0.48              |
| 1:E:249:LYS:HE2  | 1:E:279:MET:HE3  | 1.96                     | 0.48              |
| 1:F:38:THR:HG22  | 1:F:50:LYS:HE3   | 1.95                     | 0.48              |
| 1:F:89:GLN:HG2   | 1:F:97:THR:HA    | 1.95                     | 0.48              |
| 1:F:233:ARG:HH11 | 1:F:233:ARG:HG3  | 1.78                     | 0.48              |
| 1:F:355:LEU:HB3  | 1:F:360:MET:SD   | 2.54                     | 0.48              |
| 1:F:421:ARG:HB2  | 1:F:421:ARG:NH1  | 2.12                     | 0.48              |
| 1:F:445:LYS:C    | 1:F:448:PRO:HD2  | 2.39                     | 0.48              |
| 1:H:449:LYS:HG3  | 1:H:463:LEU:HD22 | 1.95                     | 0.48              |
| 1:A:424:GLU:OE1  | 1:A:424:GLU:HA   | 2.14                     | 0.47              |
| 1:B:37:GLU:HG2   | 1:B:40:ARG:NH1   | 2.29                     | 0.47              |
| 1:C:204:LYS:HB3  | 1:C:384:ILE:CG2  | 2.41                     | 0.47              |
| 1:E:465:LYS:O    | 1:E:469:GLU:HG2  | 2.13                     | 0.47              |
| 1:F:42:THR:HG22  | 1:F:48:MET:O     | 2.14                     | 0.47              |
| 1:G:189:LYS:HD2  | 1:G:190:ASP:N    | 2.28                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:281:ASP:OD1  | 1:G:308:TYR:OH   | 2.20                     | 0.47              |
| 1:A:333:VAL:HG21 | 1:A:339:LEU:HD13 | 1.96                     | 0.47              |
| 1:C:11:ILE:HD13  | 1:C:12:LEU:HB2   | 1.96                     | 0.47              |
| 1:E:239:ILE:HD11 | 1:E:347:ALA:CB   | 2.43                     | 0.47              |
| 1:F:53:VAL:HG21  | 1:G:77:PRO:CG    | 2.44                     | 0.47              |
| 1:F:145:ARG:HH11 | 1:F:145:ARG:HG2  | 1.79                     | 0.47              |
| 1:F:207:GLY:HA2  | 1:G:92:GLU:OE1   | 2.14                     | 0.47              |
| 1:F:293:VAL:HG21 | 1:F:297:ILE:HD11 | 1.96                     | 0.47              |
| 1:F:463:LEU:O    | 1:F:467:ILE:HG13 | 2.14                     | 0.47              |
| 1:G:217:ARG:HH11 | 1:G:217:ARG:CB   | 2.24                     | 0.47              |
| 1:H:281:ASP:O    | 1:H:285:GLN:HG3  | 2.14                     | 0.47              |
| 1:A:412:GLY:O    | 1:A:415:GLU:HG2  | 2.14                     | 0.47              |
| 1:B:134:LYS:O    | 1:B:138:ILE:HG13 | 2.14                     | 0.47              |
| 1:C:249:LYS:HE2  | 1:C:279:MET:CE   | 2.45                     | 0.47              |
| 1:D:125:ILE:CD1  | 1:D:517:ARG:HG2  | 2.42                     | 0.47              |
| 1:F:498:LEU:HD13 | 1:F:502:LYS:HD3  | 1.95                     | 0.47              |
| 1:G:409:PRO:HA   | 1:G:495:ILE:HG22 | 1.95                     | 0.47              |
| 1:A:230:MET:HE2  | 1:A:310:ILE:O    | 2.15                     | 0.47              |
| 1:E:120:HIS:CG   | 1:E:121:PRO:HD2  | 2.49                     | 0.47              |
| 1:H:414:PRO:HD2  | 1:H:415:GLU:OE2  | 2.15                     | 0.47              |
| 1:A:77:PRO:HB2   | 1:H:51:MET:HE3   | 1.96                     | 0.47              |
| 1:A:487:ALA:HB3  | 1:A:489:MET:CE   | 2.44                     | 0.47              |
| 1:B:91:LYS:HB2   | 1:B:91:LYS:HZ2   | 1.79                     | 0.47              |
| 1:B:241:LEU:HD22 | 1:B:330:ALA:CB   | 2.45                     | 0.47              |
| 1:E:197:LEU:HD22 | 1:E:395:VAL:HG12 | 1.96                     | 0.47              |
| 1:E:498:LEU:HD22 | 1:E:498:LEU:O    | 2.15                     | 0.47              |
| 1:G:150:ASP:OD1  | 1:G:153:THR:HG23 | 2.14                     | 0.47              |
| 1:G:481:VAL:HG22 | 3:G:7528:ADP:N1  | 2.29                     | 0.47              |
| 1:H:184:GLN:NE2  | 1:H:217:ARG:NH2  | 2.61                     | 0.47              |
| 1:A:518:ILE:HD13 | 1:H:51:MET:HB2   | 1.96                     | 0.47              |
| 1:B:54:ASP:OD1   | 1:B:58:ASP:CB    | 2.62                     | 0.47              |
| 1:B:123:ILE:HG21 | 1:B:432:LYS:HB3  | 1.95                     | 0.47              |
| 1:C:51:MET:CE    | 1:D:77:PRO:HB2   | 2.44                     | 0.47              |
| 1:C:229:ARG:NH1  | 1:D:332:ILE:O    | 2.47                     | 0.47              |
| 1:C:286:THR:HG21 | 1:C:339:LEU:HG   | 1.95                     | 0.47              |
| 1:C:298:ASP:O    | 1:C:302:GLN:HG3  | 2.14                     | 0.47              |
| 1:F:22:ARG:CG    | 1:F:23:ASP:N     | 2.78                     | 0.47              |
| 1:F:370:LYS:HE2  | 1:F:370:LYS:CA   | 2.39                     | 0.47              |
| 1:G:91:LYS:HB2   | 1:G:91:LYS:NZ    | 2.29                     | 0.47              |
| 1:G:167:ALA:C    | 1:G:169:SER:H    | 2.23                     | 0.47              |
| 1:H:425:TYR:O    | 1:H:429:VAL:HG23 | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:257:ILE:HG12 | 1:H:259:ILE:HG21 | 1.95                     | 0.47              |
| 1:A:367:LYS:HG2  | 1:A:368:ASN:N    | 2.29                     | 0.47              |
| 1:A:514:MET:HE1  | 1:H:382:HIS:CB   | 2.45                     | 0.47              |
| 1:B:91:LYS:HG2   | 1:B:91:LYS:O     | 2.14                     | 0.47              |
| 1:B:150:ASP:OD2  | 1:B:152:GLU:HB3  | 2.14                     | 0.47              |
| 1:B:260:THR:N    | 1:B:264:GLN:HE22 | 1.86                     | 0.47              |
| 1:B:397:VAL:HG23 | 1:B:398:VAL:N    | 2.30                     | 0.47              |
| 1:B:497:PRO:HB2  | 1:B:500:VAL:HG23 | 1.95                     | 0.47              |
| 1:C:75:GLN:HG2   | 1:D:13:PRO:HD3   | 1.97                     | 0.47              |
| 1:C:82:MET:CE    | 1:C:101:VAL:HG13 | 2.43                     | 0.47              |
| 1:C:94:GLY:CA    | 1:C:396:LYS:HD2  | 2.45                     | 0.47              |
| 1:C:276:LEU:HD23 | 1:C:300:LEU:HB2  | 1.97                     | 0.47              |
| 1:D:51:MET:CE    | 1:E:77:PRO:HB2   | 2.44                     | 0.47              |
| 1:E:103:ILE:O    | 1:E:103:ILE:HG22 | 2.14                     | 0.47              |
| 1:F:26:ARG:HH11  | 1:F:26:ARG:HB3   | 1.78                     | 0.47              |
| 1:F:37:GLU:HG2   | 1:F:40:ARG:NH1   | 2.30                     | 0.47              |
| 1:F:222:ASP:O    | 1:F:223:LYS:HG2  | 2.15                     | 0.47              |
| 1:G:59:ILE:HD11  | 1:H:80:LYS:HE2   | 1.96                     | 0.47              |
| 1:G:188:LYS:HB2  | 1:G:193:TYR:HA   | 1.97                     | 0.47              |
| 1:G:227:HIS:HE2  | 1:H:334:THR:CB   | 2.26                     | 0.47              |
| 1:G:269:LEU:CD1  | 1:H:251:THR:HG23 | 2.44                     | 0.47              |
| 1:H:13:PRO:O     | 1:H:16:THR:HB    | 2.15                     | 0.47              |
| 1:H:18:ARG:HA    | 1:H:521:VAL:O    | 2.15                     | 0.47              |
| 1:H:294:GLN:HB2  | 1:H:321:MET:HE2  | 1.97                     | 0.47              |
| 1:A:370:LYS:HE2  | 1:A:370:LYS:CA   | 2.40                     | 0.47              |
| 1:B:208:GLU:HB3  | 1:B:212:GLU:CG   | 2.44                     | 0.47              |
| 1:D:413:ALA:HB3  | 1:D:414:PRO:HD3  | 1.95                     | 0.47              |
| 1:F:205:LYS:HZ3  | 1:F:358:GLU:HB2  | 1.80                     | 0.47              |
| 1:C:106:GLU:HB2  | 1:C:446:ILE:HG12 | 1.97                     | 0.47              |
| 1:C:208:GLU:OE2  | 1:C:212:GLU:HG3  | 2.15                     | 0.47              |
| 1:D:16:THR:HA    | 1:D:523:ALA:O    | 2.15                     | 0.47              |
| 1:D:38:THR:O     | 1:D:50:LYS:HE3   | 2.15                     | 0.47              |
| 1:D:215:LEU:HD11 | 1:D:372:VAL:CG2  | 2.45                     | 0.47              |
| 1:D:283:ILE:HA   | 1:D:339:LEU:HD23 | 1.96                     | 0.47              |
| 1:G:241:LEU:HD22 | 1:G:330:ALA:HB3  | 1.97                     | 0.47              |
| 1:G:462:MET:CE   | 1:G:486:PRO:HD3  | 2.42                     | 0.47              |
| 1:H:208:GLU:HB3  | 1:H:212:GLU:HG3  | 1.95                     | 0.47              |
| 1:B:99:THR:O     | 1:B:103:ILE:HG13 | 2.14                     | 0.47              |
| 1:C:144:ILE:CD1  | 1:C:490:LEU:HD21 | 2.39                     | 0.47              |
| 1:D:25:GLN:O     | 1:D:29:ILE:HG13  | 2.15                     | 0.47              |
| 1:D:92:GLU:O     | 1:D:499:ARG:HD3  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:29:ILE:HG23  | 1:E:108:LEU:HB3  | 1.97                     | 0.47              |
| 1:E:269:LEU:CD1  | 1:F:251:THR:HG23 | 2.45                     | 0.47              |
| 1:G:120:HIS:ND1  | 1:G:122:SER:HB3  | 2.30                     | 0.47              |
| 1:H:91:LYS:HG2   | 1:H:91:LYS:O     | 2.15                     | 0.47              |
| 1:H:150:ASP:OD1  | 1:H:153:THR:HG23 | 2.14                     | 0.47              |
| 1:H:433:GLU:CD   | 1:H:433:GLU:H    | 2.22                     | 0.47              |
| 1:A:146:VAL:HG21 | 1:A:153:THR:HG21 | 1.97                     | 0.46              |
| 1:A:370:LYS:HA   | 1:A:370:LYS:CE   | 2.40                     | 0.46              |
| 1:B:126:LYS:O    | 1:B:130:LEU:HG   | 2.14                     | 0.46              |
| 1:B:250:LYS:HZ3  | 1:C:253:THR:HA   | 1.79                     | 0.46              |
| 1:B:314:ARG:HD2  | 1:B:315:ARG:CD   | 2.45                     | 0.46              |
| 1:C:210:VAL:HA   | 1:C:377:ARG:O    | 2.15                     | 0.46              |
| 1:D:483:GLU:O    | 1:D:485:LYS:HG2  | 2.14                     | 0.46              |
| 1:F:446:ILE:N    | 1:F:446:ILE:HD12 | 2.29                     | 0.46              |
| 1:H:417:GLU:HG3  | 1:H:421:ARG:HH12 | 1.80                     | 0.46              |
| 1:A:221:ILE:HD11 | 1:A:324:LEU:HD11 | 1.96                     | 0.46              |
| 1:A:449:LYS:HE3  | 1:A:459:THR:HG21 | 1.98                     | 0.46              |
| 1:B:89:GLN:HG2   | 1:B:97:THR:HA    | 1.97                     | 0.46              |
| 1:C:18:ARG:HG3   | 1:C:522:ILE:HG12 | 1.98                     | 0.46              |
| 1:C:225:VAL:HG11 | 1:C:230:MET:HB2  | 1.97                     | 0.46              |
| 1:D:412:GLY:O    | 1:D:415:GLU:HG2  | 2.15                     | 0.46              |
| 1:G:15:GLY:O     | 1:G:525:LYS:HE2  | 2.14                     | 0.46              |
| 1:G:211:GLU:OE1  | 1:G:211:GLU:HA   | 2.15                     | 0.46              |
| 1:B:144:ILE:HG22 | 1:B:144:ILE:O    | 2.14                     | 0.46              |
| 1:C:35:ILE:HG13  | 1:C:74:LEU:HD13  | 1.97                     | 0.46              |
| 1:D:208:GLU:HB3  | 1:D:212:GLU:CG   | 2.45                     | 0.46              |
| 1:D:259:ILE:HG21 | 1:E:257:ILE:HG12 | 1.96                     | 0.46              |
| 1:G:239:ILE:HD12 | 1:G:239:ILE:N    | 2.30                     | 0.46              |
| 1:H:150:ASP:OD2  | 1:H:152:GLU:HB3  | 2.16                     | 0.46              |
| 1:H:209:GLY:C    | 1:H:211:GLU:H    | 2.24                     | 0.46              |
| 1:H:432:LYS:O    | 1:H:435:LEU:HB2  | 2.14                     | 0.46              |
| 1:B:372:VAL:HG22 | 1:B:373:THR:H    | 1.79                     | 0.46              |
| 1:D:75:GLN:HG3   | 1:E:10:VAL:HG13  | 1.96                     | 0.46              |
| 1:G:59:ILE:N     | 1:G:59:ILE:CD1   | 2.76                     | 0.46              |
| 1:H:11:ILE:HG23  | 1:H:12:LEU:N     | 2.30                     | 0.46              |
| 1:H:450:THR:O    | 1:H:454:ASN:ND2  | 2.48                     | 0.46              |
| 1:B:348:GLU:O    | 1:B:349:VAL:HG23 | 2.15                     | 0.46              |
| 1:C:239:ILE:HD11 | 1:C:347:ALA:HB3  | 1.98                     | 0.46              |
| 1:D:182:VAL:HG22 | 1:D:395:VAL:HG13 | 1.98                     | 0.46              |
| 1:G:35:ILE:HD11  | 1:G:74:LEU:HD22  | 1.97                     | 0.46              |
| 1:G:106:GLU:HG2  | 1:G:446:ILE:HG13 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:370:LYS:HE2  | 1:H:370:LYS:CA   | 2.43                     | 0.46              |
| 1:A:91:LYS:HB2   | 1:A:91:LYS:HZ3   | 1.79                     | 0.46              |
| 1:A:465:LYS:O    | 1:A:469:GLU:HG2  | 2.15                     | 0.46              |
| 1:B:421:ARG:HB2  | 1:B:421:ARG:NH1  | 2.21                     | 0.46              |
| 1:E:208:GLU:HB3  | 1:E:212:GLU:HG3  | 1.98                     | 0.46              |
| 1:E:229:ARG:HG2  | 1:E:229:ARG:HH11 | 1.81                     | 0.46              |
| 1:E:401:VAL:O    | 1:E:405:GLY:N    | 2.44                     | 0.46              |
| 1:F:293:VAL:CG2  | 1:F:297:ILE:HD11 | 2.46                     | 0.46              |
| 1:G:103:ILE:HG12 | 1:G:446:ILE:HD11 | 1.97                     | 0.46              |
| 1:G:271:GLN:O    | 1:G:275:MET:HG3  | 2.16                     | 0.46              |
| 1:G:286:THR:HG21 | 1:G:339:LEU:HG   | 1.97                     | 0.46              |
| 1:H:209:GLY:C    | 1:H:211:GLU:N    | 2.73                     | 0.46              |
| 1:H:426:ALA:CB   | 1:H:438:GLU:HG3  | 2.45                     | 0.46              |
| 1:A:392:GLU:O    | 1:A:396:LYS:HE3  | 2.16                     | 0.46              |
| 1:A:498:LEU:HD13 | 1:A:498:LEU:C    | 2.41                     | 0.46              |
| 1:A:524:ALA:O    | 1:A:525:LYS:HD2  | 2.16                     | 0.46              |
| 1:B:154:LEU:HD12 | 1:B:154:LEU:HA   | 1.83                     | 0.46              |
| 1:B:162:ILE:HD13 | 1:B:174:LEU:HB2  | 1.98                     | 0.46              |
| 1:D:11:ILE:HD13  | 1:D:11:ILE:O     | 2.15                     | 0.46              |
| 1:D:106:GLU:HG2  | 1:D:446:ILE:HG12 | 1.97                     | 0.46              |
| 1:E:20:VAL:O     | 1:E:23:ASP:HB2   | 2.15                     | 0.46              |
| 1:E:498:LEU:C    | 1:E:498:LEU:HD13 | 2.41                     | 0.46              |
| 1:G:103:ILE:O    | 1:G:107:LEU:HB2  | 2.16                     | 0.46              |
| 1:H:480:ASP:HB3  | 1:H:483:GLU:HB2  | 1.98                     | 0.46              |
| 1:H:498:LEU:C    | 1:H:498:LEU:HD13 | 2.40                     | 0.46              |
| 1:B:126:LYS:HB3  | 1:B:126:LYS:HZ2  | 1.80                     | 0.46              |
| 1:B:498:LEU:O    | 1:B:498:LEU:HD22 | 2.16                     | 0.46              |
| 1:C:38:THR:O     | 1:C:50:LYS:HE3   | 2.16                     | 0.46              |
| 1:C:114:LEU:HG   | 1:C:439:ASN:ND2  | 2.31                     | 0.46              |
| 1:D:29:ILE:O     | 1:D:33:ARG:HG3   | 2.15                     | 0.46              |
| 1:E:75:GLN:HB2   | 1:F:11:ILE:C     | 2.41                     | 0.46              |
| 1:H:119:ILE:HD11 | 1:H:435:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:126:LYS:HB3  | 1:A:126:LYS:HZ2  | 1.79                     | 0.46              |
| 1:A:276:LEU:HD23 | 1:A:300:LEU:CB   | 2.46                     | 0.46              |
| 1:B:443:ALA:O    | 1:B:446:ILE:HG13 | 2.16                     | 0.46              |
| 1:C:91:LYS:O     | 1:C:91:LYS:HG2   | 2.15                     | 0.46              |
| 1:C:154:LEU:HG   | 1:C:398:VAL:HG13 | 1.97                     | 0.46              |
| 1:C:458:ASP:O    | 1:C:459:THR:C    | 2.59                     | 0.46              |
| 1:E:424:GLU:O    | 1:E:428:GLN:HG2  | 2.16                     | 0.46              |
| 1:F:189:LYS:HD2  | 1:F:189:LYS:C    | 2.41                     | 0.46              |
| 1:G:147:ASP:HB3  | 1:G:150:ASP:HB2  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:514:MET:O    | 1:H:514:MET:HG2  | 2.16                     | 0.46              |
| 1:A:255:ALA:HB2  | 1:H:257:ILE:HB   | 1.98                     | 0.46              |
| 1:A:466:VAL:HG21 | 1:A:479:ILE:CG1  | 2.46                     | 0.46              |
| 1:B:11:ILE:HD13  | 1:B:11:ILE:O     | 2.16                     | 0.46              |
| 1:D:188:LYS:HD3  | 1:D:193:TYR:CD1  | 2.51                     | 0.46              |
| 1:E:126:LYS:HB3  | 1:E:126:LYS:HZ2  | 1.81                     | 0.46              |
| 1:H:91:LYS:HB2   | 1:H:91:LYS:HZ2   | 1.79                     | 0.46              |
| 1:H:195:VAL:HB   | 1:H:399:LYS:HG3  | 1.98                     | 0.46              |
| 1:A:141:GLU:C    | 1:A:143:ALA:H    | 2.23                     | 0.45              |
| 1:A:506:LYS:O    | 1:A:510:GLU:CG   | 2.63                     | 0.45              |
| 1:B:109:ARG:NH2  | 1:B:110:LYS:HD3  | 2.31                     | 0.45              |
| 1:D:38:THR:HG22  | 1:D:50:LYS:HE3   | 1.97                     | 0.45              |
| 1:D:99:THR:O     | 1:D:103:ILE:HG13 | 2.16                     | 0.45              |
| 1:D:432:LYS:O    | 1:D:435:LEU:HB2  | 2.16                     | 0.45              |
| 1:E:123:ILE:HG21 | 1:E:432:LYS:CB   | 2.46                     | 0.45              |
| 1:F:162:ILE:HG21 | 1:F:171:LYS:HA   | 1.98                     | 0.45              |
| 1:F:416:ILE:HD13 | 1:F:466:VAL:HG12 | 1.98                     | 0.45              |
| 1:H:412:GLY:O    | 1:H:416:ILE:HG13 | 2.17                     | 0.45              |
| 1:H:424:GLU:O    | 1:H:428:GLN:HG3  | 2.16                     | 0.45              |
| 1:A:252:GLU:O    | 1:H:250:LYS:NZ   | 2.47                     | 0.45              |
| 1:A:255:ALA:CB   | 1:H:257:ILE:HB   | 2.46                     | 0.45              |
| 1:C:128:TYR:CE2  | 1:C:440:PHE:HB2  | 2.51                     | 0.45              |
| 1:C:178:ALA:O    | 1:C:182:VAL:HG23 | 2.15                     | 0.45              |
| 1:D:189:LYS:HD2  | 1:D:189:LYS:C    | 2.40                     | 0.45              |
| 1:E:134:LYS:O    | 1:E:138:ILE:HG13 | 2.16                     | 0.45              |
| 1:G:82:MET:HE1   | 1:G:104:ALA:HB3  | 1.98                     | 0.45              |
| 1:A:120:HIS:ND1  | 1:A:122:SER:HB3  | 2.31                     | 0.45              |
| 1:A:469:GLU:HG3  | 1:A:486:PRO:CB   | 2.46                     | 0.45              |
| 1:B:211:GLU:OE1  | 1:B:211:GLU:HA   | 2.16                     | 0.45              |
| 1:C:369:PRO:O    | 1:C:370:LYS:HE2  | 2.16                     | 0.45              |
| 1:D:123:ILE:HG23 | 1:D:433:GLU:OE2  | 2.15                     | 0.45              |
| 1:D:188:LYS:HD2  | 1:D:191:GLY:O    | 2.17                     | 0.45              |
| 1:D:188:LYS:HG3  | 1:D:192:LYS:C    | 2.40                     | 0.45              |
| 1:D:410:ALA:HB3  | 1:D:494:ILE:HG22 | 1.97                     | 0.45              |
| 1:E:243:ASN:OD1  | 1:E:295:LYS:HE3  | 2.16                     | 0.45              |
| 1:E:245:ALA:HB1  | 1:E:247:GLU:HG2  | 1.97                     | 0.45              |
| 1:E:469:GLU:HA   | 1:E:469:GLU:OE2  | 2.16                     | 0.45              |
| 1:F:120:HIS:ND1  | 1:F:121:PRO:HD2  | 2.31                     | 0.45              |
| 1:G:488:ASP:O    | 1:G:492:LYS:HG2  | 2.16                     | 0.45              |
| 1:H:12:LEU:HD23  | 1:H:13:PRO:HD2   | 1.96                     | 0.45              |
| 1:H:139:LEU:HD23 | 1:H:142:ILE:HD11 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:37:GLU:HA    | 1:A:40:ARG:HG2   | 1.97                     | 0.45              |
| 1:A:54:ASP:OD1   | 1:A:58:ASP:HB3   | 2.15                     | 0.45              |
| 1:C:418:LEU:O    | 1:C:422:LEU:HB2  | 2.16                     | 0.45              |
| 1:D:35:ILE:HD11  | 1:D:74:LEU:HD22  | 1.98                     | 0.45              |
| 1:D:38:THR:O     | 1:D:50:LYS:CE    | 2.64                     | 0.45              |
| 1:E:466:VAL:HG21 | 1:E:479:ILE:CG1  | 2.46                     | 0.45              |
| 1:E:469:GLU:O    | 1:E:473:ARG:N    | 2.48                     | 0.45              |
| 1:F:259:ILE:HD12 | 1:F:259:ILE:N    | 2.30                     | 0.45              |
| 1:G:182:VAL:O    | 1:G:186:ALA:HB2  | 2.16                     | 0.45              |
| 1:G:290:VAL:HG22 | 1:G:311:MET:HE2  | 1.99                     | 0.45              |
| 1:G:524:ALA:C    | 1:G:525:LYS:HD2  | 2.42                     | 0.45              |
| 1:H:142:ILE:HB   | 1:H:475:LEU:HD22 | 1.99                     | 0.45              |
| 1:H:149:ASP:O    | 1:H:151:GLU:N    | 2.49                     | 0.45              |
| 1:H:297:ILE:HD12 | 1:H:314:ARG:HB3  | 1.98                     | 0.45              |
| 1:B:293:VAL:CG2  | 1:B:297:ILE:HD11 | 2.46                     | 0.45              |
| 1:C:91:LYS:HB2   | 1:C:91:LYS:NZ    | 2.31                     | 0.45              |
| 1:D:462:MET:HE2  | 1:D:466:VAL:CG2  | 2.46                     | 0.45              |
| 1:D:483:GLU:HG3  | 1:D:485:LYS:CE   | 2.47                     | 0.45              |
| 1:E:136:GLN:HA   | 1:E:136:GLN:HE21 | 1.81                     | 0.45              |
| 1:E:208:GLU:HB3  | 1:E:212:GLU:HG2  | 1.98                     | 0.45              |
| 1:G:313:VAL:HG21 | 1:G:361:ILE:CD1  | 2.47                     | 0.45              |
| 1:G:449:LYS:HG3  | 1:G:463:LEU:HD22 | 1.98                     | 0.45              |
| 1:G:470:HIS:HA   | 1:G:477:ILE:HB   | 1.99                     | 0.45              |
| 1:H:114:LEU:HD11 | 1:H:436:ALA:HA   | 1.98                     | 0.45              |
| 1:H:204:LYS:HD2  | 1:H:384:ILE:HG22 | 1.99                     | 0.45              |
| 1:A:77:PRO:HG2   | 1:H:53:VAL:HG21  | 1.98                     | 0.45              |
| 1:D:195:VAL:HB   | 1:D:399:LYS:HG3  | 1.98                     | 0.45              |
| 1:E:145:ARG:HD3  | 1:E:145:ARG:HA   | 1.76                     | 0.45              |
| 1:E:394:ALA:O    | 1:E:397:VAL:CG2  | 2.65                     | 0.45              |
| 1:F:201:LYS:HE2  | 1:F:203:GLU:OE1  | 2.17                     | 0.45              |
| 1:F:241:LEU:HD12 | 1:F:292:PHE:HB2  | 1.98                     | 0.45              |
| 1:F:276:LEU:CD2  | 1:F:300:LEU:HB2  | 2.43                     | 0.45              |
| 1:G:146:VAL:HG21 | 1:G:153:THR:HG21 | 1.99                     | 0.45              |
| 1:G:205:LYS:O    | 1:G:377:ARG:NH1  | 2.49                     | 0.45              |
| 1:G:393:ASP:O    | 1:G:397:VAL:HG13 | 2.17                     | 0.45              |
| 1:H:463:LEU:O    | 1:H:467:ILE:HG13 | 2.17                     | 0.45              |
| 1:A:76:HIS:CD2   | 1:A:78:ALA:H     | 2.35                     | 0.45              |
| 1:B:17:GLN:NE2   | 1:B:17:GLN:H     | 2.15                     | 0.45              |
| 1:B:123:ILE:HG21 | 1:B:432:LYS:CB   | 2.47                     | 0.45              |
| 1:C:222:ASP:OD1  | 1:C:360:MET:HE3  | 2.17                     | 0.45              |
| 1:D:12:LEU:CD2   | 1:D:16:THR:HG21  | 2.43                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:35:ILE:HD13  | 1:D:35:ILE:HA    | 1.80                     | 0.45              |
| 1:F:408:LEU:HD11 | 1:F:498:LEU:HD23 | 1.99                     | 0.45              |
| 1:G:90:ASP:O     | 1:G:94:GLY:HA2   | 2.17                     | 0.45              |
| 1:G:109:ARG:NH2  | 1:G:110:LYS:HD3  | 2.32                     | 0.45              |
| 1:G:110:LYS:HE3  | 1:G:442:ASP:OD1  | 2.17                     | 0.45              |
| 1:H:45:PRO:HB2   | 1:H:481:VAL:HG21 | 1.99                     | 0.45              |
| 1:A:35:ILE:HD13  | 1:A:35:ILE:HA    | 1.82                     | 0.45              |
| 1:B:215:LEU:HD11 | 1:B:372:VAL:CG2  | 2.47                     | 0.45              |
| 1:B:243:ASN:O    | 1:B:243:ASN:CG   | 2.59                     | 0.45              |
| 1:B:265:LEU:O    | 1:B:269:LEU:HD13 | 2.16                     | 0.45              |
| 1:C:262:PRO:O    | 1:D:271:GLN:HG2  | 2.17                     | 0.45              |
| 1:D:235:GLU:O    | 1:D:348:GLU:O    | 2.35                     | 0.45              |
| 1:E:76:HIS:HB2   | 1:F:11:ILE:HA    | 1.98                     | 0.45              |
| 1:E:414:PRO:HD2  | 1:E:415:GLU:OE2  | 2.17                     | 0.45              |
| 1:G:410:ALA:O    | 1:G:489:MET:HG3  | 2.17                     | 0.45              |
| 1:H:260:THR:N    | 1:H:264:GLN:HE22 | 1.99                     | 0.45              |
| 1:H:372:VAL:CG2  | 1:H:373:THR:N    | 2.79                     | 0.45              |
| 1:B:69:LEU:HB3   | 1:B:83:VAL:HG22  | 1.98                     | 0.45              |
| 1:C:89:GLN:HG2   | 1:C:97:THR:HA    | 1.98                     | 0.45              |
| 1:C:143:ALA:HB3  | 1:C:145:ARG:NH1  | 2.31                     | 0.45              |
| 1:C:355:LEU:O    | 1:C:356:ALA:HB3  | 2.17                     | 0.45              |
| 1:D:241:LEU:HD12 | 1:D:292:PHE:HB2  | 1.99                     | 0.45              |
| 1:E:269:LEU:HD12 | 1:F:251:THR:CG2  | 2.43                     | 0.45              |
| 1:F:167:ALA:O    | 1:F:169:SER:N    | 2.50                     | 0.45              |
| 1:G:75:GLN:HB2   | 1:H:11:ILE:C     | 2.42                     | 0.45              |
| 1:G:215:LEU:HD11 | 1:G:372:VAL:CG2  | 2.47                     | 0.45              |
| 1:G:222:ASP:OD1  | 1:G:360:MET:HE3  | 2.16                     | 0.45              |
| 1:A:25:GLN:O     | 1:A:29:ILE:HG13  | 2.16                     | 0.45              |
| 1:A:37:GLU:HG2   | 1:A:40:ARG:CZ    | 2.47                     | 0.45              |
| 1:A:117:GLN:O    | 1:A:118:ASN:HB2  | 2.16                     | 0.45              |
| 1:A:141:GLU:O    | 1:A:143:ALA:N    | 2.50                     | 0.45              |
| 1:A:210:VAL:HA   | 1:A:377:ARG:O    | 2.16                     | 0.45              |
| 1:A:503:GLN:NE2  | 1:A:503:GLN:HA   | 2.32                     | 0.45              |
| 1:C:356:ALA:C    | 1:C:358:GLU:H    | 2.24                     | 0.45              |
| 1:C:412:GLY:HA2  | 1:C:415:GLU:CG   | 2.47                     | 0.45              |
| 1:E:116:ASP:C    | 1:E:118:ASN:H    | 2.24                     | 0.45              |
| 1:E:227:HIS:HD2  | 1:E:302:GLN:HB3  | 1.82                     | 0.45              |
| 1:E:286:THR:HG22 | 1:E:341:PRO:CD   | 2.47                     | 0.45              |
| 1:E:335:ASN:ND2  | 1:E:337:LYS:HB2  | 2.30                     | 0.45              |
| 1:F:409:PRO:HB2  | 1:F:489:MET:HB2  | 1.99                     | 0.45              |
| 1:G:17:GLN:H     | 1:G:17:GLN:HE21  | 1.62                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:152:GLU:CD   | 1:G:156:LYS:HE3  | 2.42                     | 0.45              |
| 1:G:445:LYS:C    | 1:G:448:PRO:HD2  | 2.42                     | 0.45              |
| 1:A:215:LEU:HD11 | 1:A:372:VAL:CG2  | 2.47                     | 0.44              |
| 1:B:29:ILE:HG23  | 1:B:108:LEU:HB3  | 1.97                     | 0.44              |
| 1:B:218:GLY:HA3  | 1:B:363:VAL:O    | 2.16                     | 0.44              |
| 1:B:353:ARG:HD2  | 1:B:362:PHE:CD1  | 2.52                     | 0.44              |
| 1:C:52:LEU:HD11  | 1:C:68:ILE:HA    | 1.98                     | 0.44              |
| 1:C:415:GLU:HG3  | 1:C:447:ILE:HB   | 1.99                     | 0.44              |
| 1:D:144:ILE:CD1  | 1:D:490:LEU:HD21 | 2.45                     | 0.44              |
| 1:D:207:GLY:O    | 1:D:208:GLU:HB2  | 2.16                     | 0.44              |
| 1:E:17:GLN:NE2   | 1:E:17:GLN:N     | 2.63                     | 0.44              |
| 1:E:157:ILE:HD11 | 1:E:495:ILE:HD12 | 2.00                     | 0.44              |
| 1:E:462:MET:HE1  | 1:E:485:LYS:HA   | 1.98                     | 0.44              |
| 1:F:206:ALA:HA   | 1:F:384:ILE:CD1  | 2.47                     | 0.44              |
| 1:F:225:VAL:HG23 | 1:F:352:GLU:OE1  | 2.18                     | 0.44              |
| 1:F:397:VAL:HG23 | 1:F:398:VAL:N    | 2.31                     | 0.44              |
| 1:F:412:GLY:C    | 1:F:415:GLU:HG2  | 2.42                     | 0.44              |
| 1:H:11:ILE:HD13  | 1:H:12:LEU:HB2   | 1.99                     | 0.44              |
| 1:H:273:GLU:HG2  | 1:H:300:LEU:HD13 | 1.99                     | 0.44              |
| 1:A:281:ASP:OD1  | 1:A:308:TYR:OH   | 2.17                     | 0.44              |
| 1:B:221:ILE:HD11 | 1:B:324:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:182:VAL:CG2  | 1:C:395:VAL:HG13 | 2.47                     | 0.44              |
| 1:D:13:PRO:O     | 1:D:16:THR:HB    | 2.17                     | 0.44              |
| 1:D:57:GLY:O     | 1:D:58:ASP:C     | 2.60                     | 0.44              |
| 1:E:38:THR:O     | 1:E:50:LYS:CE    | 2.64                     | 0.44              |
| 1:E:85:VAL:HG13  | 1:E:507:SER:HB3  | 1.99                     | 0.44              |
| 1:E:144:ILE:CD1  | 1:E:490:LEU:HD21 | 2.47                     | 0.44              |
| 1:E:216:VAL:O    | 1:E:372:VAL:HG23 | 2.17                     | 0.44              |
| 1:E:462:MET:HE3  | 1:E:462:MET:HA   | 1.99                     | 0.44              |
| 1:F:136:GLN:NE2  | 1:F:136:GLN:HA   | 2.33                     | 0.44              |
| 1:F:158:ALA:HB2  | 1:F:398:VAL:CG2  | 2.48                     | 0.44              |
| 1:F:333:VAL:HG12 | 1:F:335:ASN:H    | 1.82                     | 0.44              |
| 1:G:205:LYS:HD3  | 1:G:205:LYS:HA   | 1.74                     | 0.44              |
| 1:G:461:GLU:HG2  | 1:G:465:LYS:NZ   | 2.32                     | 0.44              |
| 1:H:52:LEU:HD11  | 1:H:68:ILE:HA    | 1.98                     | 0.44              |
| 1:H:230:MET:HE2  | 1:H:310:ILE:O    | 2.17                     | 0.44              |
| 1:A:142:ILE:HB   | 1:A:475:LEU:HD22 | 1.99                     | 0.44              |
| 1:C:212:GLU:HB2  | 1:C:377:ARG:HG3  | 2.00                     | 0.44              |
| 1:C:333:VAL:HG21 | 1:C:339:LEU:CD1  | 2.47                     | 0.44              |
| 1:C:498:LEU:O    | 1:C:498:LEU:HD22 | 2.17                     | 0.44              |
| 1:D:145:ARG:HG2  | 1:D:145:ARG:HH11 | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:446:ILE:H    | 1:E:446:ILE:CD1  | 2.28                     | 0.44              |
| 1:G:184:GLN:NE2  | 1:G:217:ARG:HH21 | 2.15                     | 0.44              |
| 1:H:108:LEU:HD11 | 1:H:515:ILE:HD12 | 1.99                     | 0.44              |
| 1:A:145:ARG:HG2  | 1:A:145:ARG:NH1  | 2.28                     | 0.44              |
| 1:B:245:ALA:HB1  | 1:B:247:GLU:HG2  | 1.98                     | 0.44              |
| 1:C:449:LYS:HE3  | 1:C:459:THR:CG2  | 2.48                     | 0.44              |
| 1:D:217:ARG:NH1  | 1:D:217:ARG:CB   | 2.74                     | 0.44              |
| 1:F:412:GLY:O    | 1:F:416:ILE:HG13 | 2.17                     | 0.44              |
| 1:G:48:MET:HA    | 1:G:48:MET:HE2   | 1.99                     | 0.44              |
| 1:G:218:GLY:HA3  | 1:G:363:VAL:O    | 2.17                     | 0.44              |
| 1:G:354:LYS:HE2  | 1:G:357:GLY:HA2  | 2.00                     | 0.44              |
| 1:G:517:ARG:HE   | 1:G:517:ARG:HB3  | 1.65                     | 0.44              |
| 1:A:18:ARG:HA    | 1:A:521:VAL:O    | 2.17                     | 0.44              |
| 1:A:251:THR:CG2  | 1:H:269:LEU:HD12 | 2.45                     | 0.44              |
| 1:B:11:ILE:C     | 1:B:11:ILE:CD1   | 2.90                     | 0.44              |
| 1:B:136:GLN:HE21 | 1:B:502:LYS:NZ   | 2.14                     | 0.44              |
| 1:B:446:ILE:HD12 | 1:B:446:ILE:N    | 2.33                     | 0.44              |
| 1:C:227:HIS:HB3  | 1:C:230:MET:SD   | 2.57                     | 0.44              |
| 1:D:215:LEU:HD11 | 1:D:372:VAL:HG21 | 2.00                     | 0.44              |
| 1:E:488:ASP:OD1  | 1:E:490:LEU:HB2  | 2.16                     | 0.44              |
| 1:F:167:ALA:C    | 1:F:169:SER:H    | 2.26                     | 0.44              |
| 1:G:140:ASP:OD1  | 1:G:502:LYS:HD2  | 2.17                     | 0.44              |
| 1:G:145:ARG:HG2  | 1:G:145:ARG:NH1  | 2.30                     | 0.44              |
| 1:G:151:GLU:O    | 1:G:155:LEU:HD23 | 2.17                     | 0.44              |
| 1:H:37:GLU:HG2   | 1:H:40:ARG:HH12  | 1.79                     | 0.44              |
| 1:H:112:GLU:HA   | 1:H:115:LEU:HD12 | 2.00                     | 0.44              |
| 1:H:147:ASP:HB3  | 1:H:150:ASP:HB2  | 1.99                     | 0.44              |
| 1:A:142:ILE:HB   | 1:A:475:LEU:CD2  | 2.48                     | 0.44              |
| 1:A:204:LYS:HD2  | 1:A:384:ILE:CG2  | 2.40                     | 0.44              |
| 1:A:209:GLY:O    | 1:A:212:GLU:HG2  | 2.17                     | 0.44              |
| 1:A:216:VAL:C    | 1:A:218:GLY:H    | 2.25                     | 0.44              |
| 1:B:35:ILE:HD12  | 1:B:69:LEU:CD2   | 2.47                     | 0.44              |
| 1:B:96:GLY:HA2   | 3:B:2528:ADP:O1B | 2.18                     | 0.44              |
| 1:B:294:GLN:HB2  | 1:B:321:MET:HE2  | 1.99                     | 0.44              |
| 1:C:202:PHE:CE2  | 1:C:374:ILE:HD12 | 2.53                     | 0.44              |
| 1:D:154:LEU:HG   | 1:D:398:VAL:HG13 | 1.99                     | 0.44              |
| 1:E:10:VAL:CG2   | 1:E:11:ILE:N     | 2.72                     | 0.44              |
| 1:E:11:ILE:HG23  | 1:E:12:LEU:N     | 2.33                     | 0.44              |
| 1:E:149:ASP:O    | 1:E:151:GLU:N    | 2.50                     | 0.44              |
| 1:F:35:ILE:HD13  | 1:F:35:ILE:HA    | 1.78                     | 0.44              |
| 1:F:205:LYS:HB3  | 1:F:377:ARG:NH1  | 2.33                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:313:VAL:HG21 | 1:F:361:ILE:CD1  | 2.46                     | 0.44              |
| 1:G:424:GLU:OE1  | 1:G:424:GLU:HA   | 2.17                     | 0.44              |
| 1:H:217:ARG:HB3  | 1:H:217:ARG:NH1  | 2.32                     | 0.44              |
| 1:H:264:GLN:O    | 1:H:265:LEU:C    | 2.61                     | 0.44              |
| 1:B:12:LEU:HD23  | 1:B:13:PRO:HD2   | 1.99                     | 0.44              |
| 1:B:146:VAL:O    | 1:B:148:PRO:HD3  | 2.18                     | 0.44              |
| 1:B:204:LYS:O    | 1:B:205:LYS:HD3  | 2.18                     | 0.44              |
| 1:B:416:ILE:CD1  | 1:B:466:VAL:HG12 | 2.48                     | 0.44              |
| 1:D:319:SER:O    | 1:D:323:LYS:HG3  | 2.18                     | 0.44              |
| 1:E:445:LYS:C    | 1:E:448:PRO:HD2  | 2.43                     | 0.44              |
| 1:F:12:LEU:HD21  | 1:F:16:THR:HG21  | 2.00                     | 0.44              |
| 1:F:284:ALA:HB2  | 1:F:308:TYR:CD1  | 2.52                     | 0.44              |
| 1:F:372:VAL:HG22 | 1:F:373:THR:N    | 2.33                     | 0.44              |
| 1:F:415:GLU:HG3  | 1:F:447:ILE:HB   | 1.99                     | 0.44              |
| 1:A:65:CYS:HB3   | 1:A:97:THR:OG1   | 2.17                     | 0.44              |
| 1:A:277:LYS:HB2  | 1:A:304:TYR:CE2  | 2.52                     | 0.44              |
| 1:C:109:ARG:HG2  | 1:C:109:ARG:HH11 | 1.83                     | 0.44              |
| 1:E:182:VAL:O    | 1:E:186:ALA:HB2  | 2.18                     | 0.44              |
| 1:E:208:GLU:HB2  | 1:E:377:ARG:HB3  | 1.99                     | 0.44              |
| 1:E:468:SER:O    | 1:E:469:GLU:C    | 2.61                     | 0.44              |
| 1:F:94:GLY:HA2   | 1:F:396:LYS:HD2  | 1.99                     | 0.44              |
| 1:G:80:LYS:O     | 1:G:83:VAL:HB    | 2.17                     | 0.44              |
| 1:G:233:ARG:HH12 | 1:G:349:VAL:HG11 | 1.83                     | 0.44              |
| 1:A:59:ILE:HD11  | 1:B:80:LYS:HE2   | 1.99                     | 0.44              |
| 1:B:233:ARG:HH12 | 1:B:349:VAL:CG1  | 2.29                     | 0.44              |
| 1:B:271:GLN:O    | 1:B:275:MET:HG3  | 2.18                     | 0.44              |
| 1:B:370:LYS:HA   | 1:B:370:LYS:CE   | 2.40                     | 0.44              |
| 1:B:412:GLY:C    | 1:B:415:GLU:HG2  | 2.43                     | 0.44              |
| 1:C:450:THR:O    | 1:C:454:ASN:ND2  | 2.51                     | 0.44              |
| 1:C:483:GLU:HG3  | 1:C:485:LYS:CE   | 2.48                     | 0.44              |
| 1:D:119:ILE:HD11 | 1:D:435:LEU:HD23 | 1.99                     | 0.44              |
| 1:D:266:MET:O    | 1:D:270:GLU:HG3  | 2.18                     | 0.44              |
| 1:D:488:ASP:CG   | 1:D:491:GLU:HG3  | 2.43                     | 0.44              |
| 1:F:69:LEU:HB3   | 1:F:83:VAL:HG22  | 1.99                     | 0.44              |
| 1:F:450:THR:O    | 1:F:454:ASN:ND2  | 2.51                     | 0.44              |
| 1:H:245:ALA:HB1  | 1:H:247:GLU:CG   | 2.48                     | 0.44              |
| 1:H:297:ILE:HG22 | 1:H:302:GLN:HG3  | 2.00                     | 0.44              |
| 1:A:170:HIS:C    | 1:A:172:GLU:N    | 2.75                     | 0.43              |
| 1:A:380:THR:HG23 | 1:A:383:VAL:H    | 1.83                     | 0.43              |
| 1:A:425:TYR:O    | 1:A:428:GLN:HG3  | 2.18                     | 0.43              |
| 1:D:110:LYS:HB3  | 1:D:439:ASN:HD22 | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:233:ARG:NH1  | 1:E:349:VAL:CG1  | 2.72                     | 0.43              |
| 1:F:31:ALA:CB    | 1:F:76:HIS:CD2   | 3.01                     | 0.43              |
| 1:F:146:VAL:CG2  | 1:F:147:ASP:N    | 2.81                     | 0.43              |
| 1:F:416:ILE:CD1  | 1:F:466:VAL:HG12 | 2.48                     | 0.43              |
| 1:G:75:GLN:CG    | 1:H:13:PRO:HD3   | 2.41                     | 0.43              |
| 1:G:392:GLU:O    | 1:G:396:LYS:HB2  | 2.17                     | 0.43              |
| 1:A:19:TYR:HB3   | 1:A:23:ASP:HB3   | 2.00                     | 0.43              |
| 1:A:217:ARG:HH11 | 1:A:217:ARG:CB   | 2.30                     | 0.43              |
| 1:C:17:GLN:NE2   | 1:C:17:GLN:N     | 2.59                     | 0.43              |
| 1:D:62:THR:OG1   | 1:D:63:ASN:N     | 2.51                     | 0.43              |
| 1:D:430:GLY:CA   | 1:D:434:ALA:HB2  | 2.48                     | 0.43              |
| 1:E:35:ILE:HG21  | 1:E:82:MET:CB    | 2.47                     | 0.43              |
| 1:F:290:VAL:HG13 | 1:F:311:MET:HE2  | 2.00                     | 0.43              |
| 1:G:31:ALA:CB    | 1:G:76:HIS:CD2   | 3.01                     | 0.43              |
| 1:G:392:GLU:O    | 1:G:396:LYS:HE3  | 2.18                     | 0.43              |
| 1:A:64:ASP:O     | 1:A:68:ILE:HG13  | 2.18                     | 0.43              |
| 1:A:413:ALA:N    | 1:A:414:PRO:CD   | 2.81                     | 0.43              |
| 1:C:147:ASP:O    | 1:C:149:ASP:N    | 2.51                     | 0.43              |
| 1:D:201:LYS:HB2  | 1:D:323:LYS:HE3  | 2.00                     | 0.43              |
| 1:D:220:VAL:HG11 | 1:D:360:MET:CE   | 2.48                     | 0.43              |
| 1:E:143:ALA:HB3  | 1:E:145:ARG:NH1  | 2.34                     | 0.43              |
| 1:F:467:ILE:HG22 | 1:F:471:LYS:HD2  | 1.99                     | 0.43              |
| 1:G:138:ILE:O    | 1:G:142:ILE:HG12 | 2.18                     | 0.43              |
| 1:H:25:GLN:O     | 1:H:29:ILE:HG13  | 2.17                     | 0.43              |
| 1:A:80:LYS:HE2   | 1:H:59:ILE:HD11  | 1.99                     | 0.43              |
| 1:B:82:MET:HE1   | 1:B:104:ALA:HB3  | 2.00                     | 0.43              |
| 1:B:262:PRO:HG2  | 1:C:267:SER:HB2  | 2.01                     | 0.43              |
| 1:B:483:GLU:HG3  | 1:B:485:LYS:HZ3  | 1.80                     | 0.43              |
| 1:C:221:ILE:HD11 | 1:C:324:LEU:HD11 | 2.01                     | 0.43              |
| 1:C:262:PRO:HG2  | 1:D:267:SER:HB2  | 2.00                     | 0.43              |
| 1:C:446:ILE:HA   | 1:C:449:LYS:HB2  | 2.00                     | 0.43              |
| 1:D:180:GLU:HG2  | 1:D:215:LEU:CD2  | 2.48                     | 0.43              |
| 1:D:353:ARG:NH2  | 1:D:364:GLU:OE2  | 2.52                     | 0.43              |
| 1:E:393:ASP:O    | 1:E:397:VAL:HG22 | 2.19                     | 0.43              |
| 1:F:265:LEU:O    | 1:F:269:LEU:HD13 | 2.18                     | 0.43              |
| 1:H:488:ASP:CG   | 1:H:491:GLU:HG3  | 2.44                     | 0.43              |
| 1:A:94:GLY:HA3   | 1:A:396:LYS:HB3  | 2.01                     | 0.43              |
| 1:B:103:ILE:O    | 1:B:103:ILE:HG22 | 2.18                     | 0.43              |
| 1:B:106:GLU:HG2  | 1:B:446:ILE:CG1  | 2.48                     | 0.43              |
| 1:D:524:ALA:C    | 1:D:525:LYS:HG2  | 2.43                     | 0.43              |
| 1:E:239:ILE:HD11 | 1:E:347:ALA:HB3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:446:ILE:HD12 | 1:E:446:ILE:N    | 2.33                     | 0.43              |
| 1:F:146:VAL:HG21 | 1:F:153:THR:HG21 | 1.99                     | 0.43              |
| 1:F:423:ASP:O    | 1:F:426:ALA:HB3  | 2.18                     | 0.43              |
| 1:G:106:GLU:OE1  | 1:G:106:GLU:HA   | 2.18                     | 0.43              |
| 1:H:94:GLY:HA2   | 1:H:396:LYS:HD2  | 1.99                     | 0.43              |
| 1:A:257:ILE:HG22 | 1:A:259:ILE:CD1  | 2.47                     | 0.43              |
| 1:B:155:LEU:HD22 | 1:B:179:VAL:HG21 | 1.99                     | 0.43              |
| 1:B:167:ALA:C    | 1:B:169:SER:H    | 2.26                     | 0.43              |
| 1:B:207:GLY:O    | 1:B:208:GLU:HB2  | 2.18                     | 0.43              |
| 1:C:206:ALA:CA   | 1:C:384:ILE:HD11 | 2.44                     | 0.43              |
| 1:E:286:THR:HG22 | 1:E:341:PRO:HG3  | 2.00                     | 0.43              |
| 1:E:392:GLU:O    | 1:E:396:LYS:HB2  | 2.19                     | 0.43              |
| 1:F:19:TYR:N     | 1:F:19:TYR:CD1   | 2.86                     | 0.43              |
| 1:F:20:VAL:HG12  | 1:F:21:GLY:N     | 2.33                     | 0.43              |
| 1:F:217:ARG:HB3  | 1:F:217:ARG:NH1  | 2.33                     | 0.43              |
| 1:G:412:GLY:C    | 1:G:415:GLU:HG2  | 2.43                     | 0.43              |
| 1:A:261:SER:O    | 1:A:264:GLN:HG3  | 2.19                     | 0.43              |
| 1:A:426:ALA:HB1  | 1:A:438:GLU:HG3  | 2.00                     | 0.43              |
| 1:B:147:ASP:O    | 1:B:149:ASP:N    | 2.52                     | 0.43              |
| 1:B:166:ASN:C    | 1:B:168:GLU:H    | 2.27                     | 0.43              |
| 1:C:300:LEU:HD23 | 1:C:300:LEU:HA   | 1.92                     | 0.43              |
| 1:C:333:VAL:HG21 | 1:C:339:LEU:HD13 | 2.00                     | 0.43              |
| 1:D:281:ASP:O    | 1:D:285:GLN:HG3  | 2.18                     | 0.43              |
| 1:E:297:ILE:CG2  | 1:E:302:GLN:HG3  | 2.47                     | 0.43              |
| 1:H:35:ILE:HG13  | 1:H:79:ALA:HB1   | 2.01                     | 0.43              |
| 1:H:271:GLN:O    | 1:H:275:MET:HG3  | 2.19                     | 0.43              |
| 1:H:293:VAL:CG2  | 1:H:297:ILE:HD11 | 2.49                     | 0.43              |
| 1:A:409:PRO:HB3  | 1:A:490:LEU:CD1  | 2.46                     | 0.43              |
| 1:B:149:ASP:N    | 1:B:149:ASP:OD2  | 2.50                     | 0.43              |
| 1:B:195:VAL:HB   | 1:B:399:LYS:HG3  | 2.01                     | 0.43              |
| 1:E:210:VAL:HA   | 1:E:377:ARG:O    | 2.19                     | 0.43              |
| 1:F:443:ALA:O    | 1:F:446:ILE:HG13 | 2.18                     | 0.43              |
| 1:G:443:ALA:C    | 1:G:445:LYS:H    | 2.26                     | 0.43              |
| 1:H:207:GLY:O    | 1:H:208:GLU:HB2  | 2.18                     | 0.43              |
| 1:A:17:GLN:N     | 1:A:17:GLN:NE2   | 2.67                     | 0.43              |
| 1:C:272:GLU:O    | 1:C:273:GLU:C    | 2.61                     | 0.43              |
| 1:E:126:LYS:O    | 1:E:130:LEU:HG   | 2.19                     | 0.43              |
| 1:E:204:LYS:CD   | 1:E:388:GLU:OE2  | 2.62                     | 0.43              |
| 1:E:356:ALA:C    | 1:E:358:GLU:H    | 2.27                     | 0.43              |
| 1:F:189:LYS:HD2  | 1:F:190:ASP:N    | 2.33                     | 0.43              |
| 1:F:489:MET:HE2  | 1:F:489:MET:HA   | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:469:GLU:O    | 1:H:473:ARG:N    | 2.52                     | 0.43              |
| 1:H:503:GLN:HA   | 1:H:503:GLN:NE2  | 2.33                     | 0.43              |
| 1:B:110:LYS:HE3  | 1:B:442:ASP:OD1  | 2.19                     | 0.43              |
| 1:D:205:LYS:O    | 1:D:377:ARG:NH1  | 2.51                     | 0.43              |
| 1:E:154:LEU:HD12 | 1:E:154:LEU:HA   | 1.88                     | 0.43              |
| 1:E:291:VAL:HG23 | 1:E:310:ILE:CG2  | 2.48                     | 0.43              |
| 1:F:224:GLU:O    | 1:F:313:VAL:HG13 | 2.19                     | 0.43              |
| 1:F:269:LEU:CD1  | 1:G:251:THR:HG23 | 2.40                     | 0.43              |
| 1:F:433:GLU:O    | 1:F:437:ILE:HG13 | 2.18                     | 0.43              |
| 1:H:290:VAL:HG13 | 1:H:311:MET:HE2  | 2.01                     | 0.43              |
| 1:A:314:ARG:O    | 1:A:315:ARG:C    | 2.62                     | 0.42              |
| 1:B:59:ILE:HD12  | 1:B:59:ILE:H     | 1.81                     | 0.42              |
| 1:C:182:VAL:O    | 1:C:186:ALA:HB2  | 2.19                     | 0.42              |
| 1:E:300:LEU:HD23 | 1:E:300:LEU:HA   | 1.84                     | 0.42              |
| 1:H:515:ILE:C    | 1:H:517:ARG:N    | 2.76                     | 0.42              |
| 1:C:75:GLN:HB2   | 1:D:11:ILE:CA    | 2.49                     | 0.42              |
| 1:C:196:ASP:OD1  | 1:C:198:ASP:HB2  | 2.19                     | 0.42              |
| 1:D:425:TYR:O    | 1:D:428:GLN:HG3  | 2.19                     | 0.42              |
| 1:D:517:ARG:HE   | 1:D:517:ARG:HB3  | 1.68                     | 0.42              |
| 1:E:72:ILE:HG22  | 1:E:74:LEU:HD23  | 2.01                     | 0.42              |
| 1:E:215:LEU:HD11 | 1:E:372:VAL:CG2  | 2.48                     | 0.42              |
| 1:E:217:ARG:HA   | 1:E:372:VAL:HG23 | 2.01                     | 0.42              |
| 1:E:221:ILE:HD11 | 1:E:324:LEU:HD11 | 2.00                     | 0.42              |
| 1:E:286:THR:CA   | 1:E:341:PRO:HG3  | 2.49                     | 0.42              |
| 1:E:404:ASP:OD1  | 1:E:499:ARG:HB2  | 2.18                     | 0.42              |
| 1:E:410:ALA:CB   | 1:E:494:ILE:HG22 | 2.46                     | 0.42              |
| 1:E:443:ALA:O    | 1:E:446:ILE:CD1  | 2.68                     | 0.42              |
| 1:F:50:LYS:HD2   | 1:F:68:ILE:HD13  | 2.01                     | 0.42              |
| 1:F:182:VAL:HG13 | 1:F:195:VAL:HG11 | 1.99                     | 0.42              |
| 1:G:197:LEU:HD22 | 1:G:395:VAL:CG1  | 2.49                     | 0.42              |
| 1:H:172:GLU:OE1  | 1:H:172:GLU:HA   | 2.19                     | 0.42              |
| 1:H:218:GLY:HA3  | 1:H:363:VAL:O    | 2.19                     | 0.42              |
| 1:H:446:ILE:O    | 1:H:450:THR:HG23 | 2.19                     | 0.42              |
| 1:A:269:LEU:CD1  | 1:B:251:THR:HG23 | 2.42                     | 0.42              |
| 1:A:348:GLU:HB3  | 1:A:365:GLY:HA3  | 2.00                     | 0.42              |
| 1:B:72:ILE:HG22  | 1:B:74:LEU:HD23  | 2.02                     | 0.42              |
| 1:C:114:LEU:HD11 | 1:C:436:ALA:HA   | 2.01                     | 0.42              |
| 1:C:412:GLY:C    | 1:C:415:GLU:HG2  | 2.44                     | 0.42              |
| 1:C:477:ILE:HA   | 1:C:487:ALA:O    | 2.19                     | 0.42              |
| 1:E:150:ASP:OD2  | 1:E:150:ASP:C    | 2.62                     | 0.42              |
| 1:A:20:VAL:HG12  | 1:A:21:GLY:N     | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:391:LEU:O    | 1:A:394:ALA:HB3  | 2.19                     | 0.42              |
| 1:B:17:GLN:H     | 1:B:17:GLN:HE21  | 1.67                     | 0.42              |
| 1:B:144:ILE:CD1  | 1:B:490:LEU:HD21 | 2.47                     | 0.42              |
| 1:C:397:VAL:HG23 | 1:C:398:VAL:N    | 2.34                     | 0.42              |
| 1:C:449:LYS:HE2  | 1:C:449:LYS:HB3  | 1.85                     | 0.42              |
| 1:D:180:GLU:CD   | 1:D:215:LEU:HD23 | 2.45                     | 0.42              |
| 1:E:37:GLU:HG2   | 1:E:40:ARG:CZ    | 2.49                     | 0.42              |
| 1:E:503:GLN:HA   | 1:E:503:GLN:HE21 | 1.84                     | 0.42              |
| 1:E:524:ALA:O    | 1:E:525:LYS:HD3  | 2.19                     | 0.42              |
| 1:F:146:VAL:CG2  | 1:F:147:ASP:H    | 2.32                     | 0.42              |
| 1:F:197:LEU:HD22 | 1:F:395:VAL:HG12 | 2.01                     | 0.42              |
| 1:F:245:ALA:HB1  | 1:F:247:GLU:HG2  | 2.01                     | 0.42              |
| 1:F:503:GLN:NE2  | 1:F:506:LYS:HD2  | 2.35                     | 0.42              |
| 1:H:52:LEU:HD13  | 1:H:71:LYS:HB2   | 2.02                     | 0.42              |
| 1:H:342:GLU:CD   | 1:H:342:GLU:N    | 2.77                     | 0.42              |
| 1:A:23:ASP:O     | 1:A:27:LEU:HG    | 2.19                     | 0.42              |
| 1:A:94:GLY:HA2   | 1:A:396:LYS:HD2  | 2.00                     | 0.42              |
| 1:C:29:ILE:HG23  | 1:C:108:LEU:HB3  | 2.01                     | 0.42              |
| 1:C:209:GLY:H    | 1:C:212:GLU:HG2  | 1.83                     | 0.42              |
| 1:C:259:ILE:HG12 | 1:C:265:LEU:HD23 | 2.02                     | 0.42              |
| 1:C:261:SER:H    | 1:C:264:GLN:HG3  | 1.83                     | 0.42              |
| 1:D:74:LEU:HD13  | 1:D:79:ALA:HB1   | 2.01                     | 0.42              |
| 1:D:138:ILE:O    | 1:D:142:ILE:HG12 | 2.20                     | 0.42              |
| 1:D:144:ILE:O    | 1:D:144:ILE:HG22 | 2.19                     | 0.42              |
| 1:E:220:VAL:CG1  | 1:E:360:MET:HE2  | 2.50                     | 0.42              |
| 1:E:276:LEU:HD23 | 1:E:300:LEU:CB   | 2.46                     | 0.42              |
| 1:F:72:ILE:HG22  | 1:F:74:LEU:CD2   | 2.50                     | 0.42              |
| 1:F:109:ARG:HG2  | 1:F:109:ARG:HH11 | 1.84                     | 0.42              |
| 1:F:112:GLU:HA   | 1:F:115:LEU:HD12 | 2.00                     | 0.42              |
| 1:F:116:ASP:C    | 1:F:118:ASN:N    | 2.76                     | 0.42              |
| 1:G:293:VAL:HG21 | 1:G:297:ILE:HD11 | 2.01                     | 0.42              |
| 1:H:91:LYS:O     | 1:H:91:LYS:CG    | 2.67                     | 0.42              |
| 1:H:272:GLU:HA   | 1:H:275:MET:CE   | 2.43                     | 0.42              |
| 1:C:270:GLU:HA   | 1:C:273:GLU:HG3  | 2.02                     | 0.42              |
| 1:E:250:LYS:NZ   | 1:F:253:THR:HA   | 2.35                     | 0.42              |
| 1:G:480:ASP:HB2  | 1:G:489:MET:HE1  | 2.00                     | 0.42              |
| 1:H:109:ARG:NH2  | 1:H:110:LYS:HD3  | 2.34                     | 0.42              |
| 1:H:147:ASP:O    | 1:H:149:ASP:N    | 2.53                     | 0.42              |
| 1:H:304:TYR:O    | 1:H:308:TYR:CD1  | 2.65                     | 0.42              |
| 1:A:236:ASN:HA   | 1:A:346:TYR:HE1  | 1.85                     | 0.42              |
| 1:B:35:ILE:HD13  | 1:B:35:ILE:HA    | 1.89                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:23:ASP:O     | 1:C:27:LEU:HG    | 2.19                     | 0.42              |
| 1:D:76:HIS:HA    | 1:D:77:PRO:HD3   | 1.91                     | 0.42              |
| 1:D:116:ASP:C    | 1:D:118:ASN:H    | 2.26                     | 0.42              |
| 1:F:126:LYS:O    | 1:F:130:LEU:HG   | 2.20                     | 0.42              |
| 1:F:286:THR:HA   | 1:F:341:PRO:HG3  | 2.01                     | 0.42              |
| 1:F:467:ILE:O    | 1:F:471:LYS:HG3  | 2.20                     | 0.42              |
| 1:G:45:PRO:HB2   | 1:G:481:VAL:HG21 | 2.00                     | 0.42              |
| 1:H:498:LEU:HD22 | 1:H:498:LEU:O    | 2.19                     | 0.42              |
| 1:A:76:HIS:CD2   | 1:A:78:ALA:HB3   | 2.55                     | 0.42              |
| 1:A:143:ALA:HB3  | 1:A:145:ARG:NH1  | 2.35                     | 0.42              |
| 1:A:156:LYS:O    | 1:A:157:ILE:C    | 2.63                     | 0.42              |
| 1:A:245:ALA:HB1  | 1:A:247:GLU:HG2  | 2.00                     | 0.42              |
| 1:A:446:ILE:N    | 1:A:446:ILE:HD12 | 2.34                     | 0.42              |
| 1:A:483:GLU:HG3  | 1:A:485:LYS:HZ3  | 1.84                     | 0.42              |
| 1:D:76:HIS:CD2   | 1:D:78:ALA:HB3   | 2.55                     | 0.42              |
| 1:E:239:ILE:HG23 | 1:E:290:VAL:HG12 | 2.01                     | 0.42              |
| 1:E:348:GLU:O    | 1:E:349:VAL:HG23 | 2.19                     | 0.42              |
| 1:F:25:GLN:O     | 1:F:29:ILE:HG13  | 2.20                     | 0.42              |
| 1:F:446:ILE:HD12 | 1:F:446:ILE:H    | 1.85                     | 0.42              |
| 1:A:227:HIS:HB3  | 1:A:230:MET:SD   | 2.59                     | 0.42              |
| 1:A:469:GLU:HG3  | 1:A:486:PRO:HB2  | 2.01                     | 0.42              |
| 1:B:370:LYS:HE2  | 1:B:370:LYS:CA   | 2.42                     | 0.42              |
| 1:B:446:ILE:HD12 | 1:B:446:ILE:H    | 1.85                     | 0.42              |
| 1:D:272:GLU:HA   | 1:D:275:MET:CE   | 2.46                     | 0.42              |
| 1:G:440:PHE:C    | 1:G:440:PHE:CD2  | 2.98                     | 0.42              |
| 1:A:141:GLU:C    | 1:A:143:ALA:N    | 2.78                     | 0.42              |
| 1:C:37:GLU:HA    | 1:C:40:ARG:HG2   | 2.01                     | 0.42              |
| 1:C:277:LYS:HB2  | 1:C:304:TYR:CE2  | 2.55                     | 0.42              |
| 1:C:315:ARG:NH1  | 1:C:315:ARG:CG   | 2.82                     | 0.42              |
| 1:C:409:PRO:HA   | 1:C:495:ILE:HG22 | 2.02                     | 0.42              |
| 1:E:114:LEU:HD22 | 1:E:119:ILE:HD12 | 2.00                     | 0.42              |
| 1:E:117:GLN:O    | 1:E:118:ASN:HB2  | 2.19                     | 0.42              |
| 1:E:152:GLU:HG3  | 1:E:153:THR:N    | 2.34                     | 0.42              |
| 1:E:188:LYS:HD3  | 1:E:193:TYR:CE1  | 2.54                     | 0.42              |
| 1:E:233:ARG:HG3  | 1:E:233:ARG:NH1  | 2.32                     | 0.42              |
| 1:F:37:GLU:HA    | 1:F:40:ARG:HG2   | 2.01                     | 0.42              |
| 1:F:342:GLU:OE2  | 1:F:342:GLU:N    | 2.50                     | 0.42              |
| 1:G:37:GLU:HA    | 1:G:40:ARG:HG2   | 2.01                     | 0.42              |
| 1:G:227:HIS:HA   | 1:G:228:PRO:HD3  | 1.91                     | 0.42              |
| 1:H:197:LEU:HD22 | 1:H:395:VAL:CG1  | 2.50                     | 0.42              |
| 1:H:370:LYS:HA   | 1:H:370:LYS:CE   | 2.45                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:40:ARG:HE    | 1:D:450:THR:HG21 | 1.85                     | 0.41              |
| 1:F:250:LYS:NZ   | 1:G:253:THR:HA   | 2.34                     | 0.41              |
| 1:F:330:ALA:HB2  | 1:F:345:GLY:HA3  | 2.01                     | 0.41              |
| 1:G:204:LYS:HD3  | 1:G:388:GLU:OE2  | 2.19                     | 0.41              |
| 1:G:481:VAL:HG13 | 3:G:7528:ADP:C2  | 2.55                     | 0.41              |
| 1:H:412:GLY:O    | 1:H:415:GLU:HG2  | 2.20                     | 0.41              |
| 1:C:51:MET:HB2   | 1:D:518:ILE:HD13 | 2.01                     | 0.41              |
| 1:D:208:GLU:HB3  | 1:D:212:GLU:HG3  | 2.01                     | 0.41              |
| 1:D:292:PHE:CE2  | 1:D:313:VAL:HG21 | 2.56                     | 0.41              |
| 1:E:144:ILE:O    | 1:E:144:ILE:HG22 | 2.19                     | 0.41              |
| 1:E:210:VAL:O    | 1:E:210:VAL:HG12 | 2.20                     | 0.41              |
| 1:G:208:GLU:CG   | 1:G:377:ARG:HH21 | 2.33                     | 0.41              |
| 1:G:412:GLY:HA2  | 1:G:415:GLU:CG   | 2.50                     | 0.41              |
| 1:A:17:GLN:NE2   | 1:A:17:GLN:H     | 2.18                     | 0.41              |
| 1:A:401:VAL:O    | 1:A:405:GLY:N    | 2.51                     | 0.41              |
| 1:B:106:GLU:CB   | 1:B:446:ILE:HG12 | 2.51                     | 0.41              |
| 1:C:94:GLY:HA2   | 1:C:396:LYS:HD2  | 2.01                     | 0.41              |
| 1:C:207:GLY:O    | 1:C:208:GLU:C    | 2.63                     | 0.41              |
| 1:C:462:MET:HA   | 1:C:462:MET:HE3  | 2.03                     | 0.41              |
| 1:C:469:GLU:O    | 1:C:473:ARG:N    | 2.53                     | 0.41              |
| 1:E:462:MET:HE2  | 1:E:486:PRO:HD3  | 2.01                     | 0.41              |
| 1:E:463:LEU:O    | 1:E:467:ILE:HG13 | 2.21                     | 0.41              |
| 1:F:462:MET:HA   | 1:F:462:MET:HE3  | 2.02                     | 0.41              |
| 1:G:76:HIS:CD2   | 1:G:78:ALA:HB3   | 2.55                     | 0.41              |
| 1:G:346:TYR:OH   | 1:G:348:GLU:HA   | 2.20                     | 0.41              |
| 1:A:138:ILE:O    | 1:A:142:ILE:HG12 | 2.20                     | 0.41              |
| 1:A:241:LEU:HD12 | 1:A:292:PHE:HB2  | 2.02                     | 0.41              |
| 1:A:369:PRO:O    | 1:A:370:LYS:CE   | 2.62                     | 0.41              |
| 1:A:483:GLU:OE1  | 1:A:483:GLU:HA   | 2.21                     | 0.41              |
| 1:B:346:TYR:CG   | 1:B:347:ALA:N    | 2.88                     | 0.41              |
| 1:C:114:LEU:HD22 | 1:C:119:ILE:HD12 | 2.02                     | 0.41              |
| 1:C:440:PHE:C    | 1:C:440:PHE:CD2  | 2.98                     | 0.41              |
| 1:D:145:ARG:HD3  | 1:D:145:ARG:HA   | 1.83                     | 0.41              |
| 1:D:216:VAL:O    | 1:D:372:VAL:CG2  | 2.68                     | 0.41              |
| 1:D:356:ALA:C    | 1:D:358:GLU:H    | 2.29                     | 0.41              |
| 1:D:417:GLU:OE2  | 1:D:470:HIS:NE2  | 2.42                     | 0.41              |
| 1:E:211:GLU:OE1  | 1:E:211:GLU:HA   | 2.21                     | 0.41              |
| 1:F:54:ASP:OD1   | 1:F:58:ASP:CB    | 2.64                     | 0.41              |
| 1:G:15:GLY:O     | 1:G:524:ALA:O    | 2.39                     | 0.41              |
| 1:G:167:ALA:HB2  | 1:G:387:VAL:HG22 | 2.01                     | 0.41              |
| 1:H:94:GLY:HA3   | 1:H:396:LYS:HB3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:72:ILE:HD11  | 1:B:522:ILE:HD12 | 2.02                     | 0.41              |
| 1:A:120:HIS:ND1  | 1:A:121:PRO:HD2  | 2.35                     | 0.41              |
| 1:A:293:VAL:HG21 | 1:A:297:ILE:HD11 | 2.03                     | 0.41              |
| 1:B:150:ASP:OD2  | 1:B:150:ASP:C    | 2.63                     | 0.41              |
| 1:B:293:VAL:HG21 | 1:B:297:ILE:HD11 | 2.02                     | 0.41              |
| 1:B:483:GLU:HG3  | 1:B:485:LYS:HZ1  | 1.86                     | 0.41              |
| 1:C:35:ILE:HD12  | 1:C:69:LEU:HD22  | 2.02                     | 0.41              |
| 1:D:498:LEU:HD13 | 1:D:502:LYS:HD3  | 2.02                     | 0.41              |
| 1:E:197:LEU:CD1  | 1:E:396:LYS:HG3  | 2.51                     | 0.41              |
| 1:E:359:ASN:C    | 1:E:360:MET:HG3  | 2.45                     | 0.41              |
| 1:E:420:ILE:HD13 | 1:E:471:LYS:HG3  | 2.02                     | 0.41              |
| 1:F:94:GLY:HA3   | 1:F:396:LYS:HB3  | 2.02                     | 0.41              |
| 1:F:173:LEU:O    | 1:F:176:LYS:HB3  | 2.19                     | 0.41              |
| 1:F:253:THR:O    | 1:F:254:ASP:C    | 2.64                     | 0.41              |
| 1:G:167:ALA:C    | 1:G:169:SER:N    | 2.78                     | 0.41              |
| 1:G:524:ALA:O    | 1:G:525:LYS:CD   | 2.69                     | 0.41              |
| 1:H:273:GLU:HG2  | 1:H:300:LEU:CD1  | 2.50                     | 0.41              |
| 1:A:51:MET:CE    | 1:B:77:PRO:HB2   | 2.50                     | 0.41              |
| 1:A:170:HIS:CD2  | 1:A:211:GLU:CD   | 2.98                     | 0.41              |
| 1:A:266:MET:HG2  | 1:B:271:GLN:NE2  | 2.36                     | 0.41              |
| 1:A:335:ASN:HB2  | 1:H:303:HIS:CD2  | 2.54                     | 0.41              |
| 1:B:18:ARG:C     | 1:B:19:TYR:CD1   | 2.99                     | 0.41              |
| 1:B:91:LYS:O     | 1:B:91:LYS:CG    | 2.68                     | 0.41              |
| 1:C:12:LEU:HD23  | 1:C:13:PRO:N     | 2.34                     | 0.41              |
| 1:C:201:LYS:HE2  | 1:C:203:GLU:OE1  | 2.21                     | 0.41              |
| 1:C:259:ILE:N    | 1:C:259:ILE:CD1  | 2.84                     | 0.41              |
| 1:D:212:GLU:OE2  | 1:D:212:GLU:CA   | 2.68                     | 0.41              |
| 1:D:304:TYR:O    | 1:D:308:TYR:CD1  | 2.67                     | 0.41              |
| 1:E:35:ILE:HA    | 1:E:35:ILE:HD13  | 1.85                     | 0.41              |
| 1:E:380:THR:CG2  | 1:E:383:VAL:H    | 2.28                     | 0.41              |
| 1:F:109:ARG:HG2  | 1:F:109:ARG:NH1  | 2.36                     | 0.41              |
| 1:F:470:HIS:CE1  | 1:F:475:LEU:HA   | 2.55                     | 0.41              |
| 1:G:192:LYS:HE2  | 1:G:192:LYS:HB3  | 1.87                     | 0.41              |
| 1:G:342:GLU:OE2  | 1:G:342:GLU:N    | 2.52                     | 0.41              |
| 1:A:157:ILE:HG13 | 1:A:401:VAL:HG21 | 2.03                     | 0.41              |
| 1:A:257:ILE:HG12 | 1:H:259:ILE:CG2  | 2.51                     | 0.41              |
| 1:A:291:VAL:O    | 1:A:312:ALA:HA   | 2.21                     | 0.41              |
| 1:B:142:ILE:HD13 | 1:B:417:GLU:HG2  | 2.03                     | 0.41              |
| 1:C:317:LYS:O    | 1:C:320:ASP:HB2  | 2.21                     | 0.41              |
| 1:C:409:PRO:HB2  | 1:C:489:MET:HB2  | 2.02                     | 0.41              |
| 1:D:126:LYS:O    | 1:D:130:LEU:HG   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:317:LYS:O    | 1:D:320:ASP:N    | 2.53                     | 0.41              |
| 1:D:381:GLU:O    | 1:D:384:ILE:HB   | 2.21                     | 0.41              |
| 1:D:462:MET:HE2  | 1:D:466:VAL:HG23 | 2.01                     | 0.41              |
| 1:E:21:GLY:O     | 1:E:22:ARG:C     | 2.62                     | 0.41              |
| 1:E:37:GLU:HA    | 1:E:40:ARG:HG2   | 2.03                     | 0.41              |
| 1:E:103:ILE:CG1  | 1:E:447:ILE:HD11 | 2.51                     | 0.41              |
| 1:E:170:HIS:C    | 1:E:172:GLU:N    | 2.78                     | 0.41              |
| 1:F:35:ILE:HG22  | 1:F:36:ALA:N     | 2.35                     | 0.41              |
| 1:F:154:LEU:HD12 | 1:F:154:LEU:HA   | 1.83                     | 0.41              |
| 1:H:94:GLY:CA    | 1:H:396:LYS:HD2  | 2.51                     | 0.41              |
| 1:A:12:LEU:HD13  | 1:A:16:THR:CG2   | 2.50                     | 0.41              |
| 1:B:490:LEU:CD1  | 1:B:490:LEU:N    | 2.84                     | 0.41              |
| 1:C:103:ILE:O    | 1:C:107:LEU:HB2  | 2.21                     | 0.41              |
| 1:D:72:ILE:CG2   | 1:D:73:ASP:N     | 2.83                     | 0.41              |
| 1:D:73:ASP:O     | 1:E:13:PRO:CD    | 2.64                     | 0.41              |
| 1:D:114:LEU:CD1  | 1:D:436:ALA:HA   | 2.51                     | 0.41              |
| 1:D:206:ALA:CA   | 1:D:384:ILE:HD11 | 2.47                     | 0.41              |
| 1:E:146:VAL:HG21 | 1:E:153:THR:HG21 | 2.03                     | 0.41              |
| 1:F:31:ALA:HB2   | 1:F:76:HIS:CD2   | 2.56                     | 0.41              |
| 1:H:227:HIS:ND1  | 1:H:228:PRO:HD2  | 2.36                     | 0.41              |
| 1:H:410:ALA:HB3  | 1:H:494:ILE:HG22 | 2.02                     | 0.41              |
| 1:A:330:ALA:HB2  | 1:A:345:GLY:HA3  | 2.03                     | 0.41              |
| 1:A:446:ILE:HD12 | 1:A:446:ILE:H    | 1.86                     | 0.41              |
| 1:B:59:ILE:N     | 1:B:59:ILE:CD1   | 2.79                     | 0.41              |
| 1:C:85:VAL:HG13  | 1:C:507:SER:HB3  | 2.02                     | 0.41              |
| 1:C:202:PHE:HE2  | 1:C:374:ILE:HD12 | 1.86                     | 0.41              |
| 1:C:216:VAL:O    | 1:C:218:GLY:N    | 2.52                     | 0.41              |
| 1:D:65:CYS:HB3   | 1:D:97:THR:OG1   | 2.21                     | 0.41              |
| 1:D:483:GLU:HG3  | 1:D:485:LYS:HE2  | 2.03                     | 0.41              |
| 1:E:165:LYS:O    | 1:E:168:GLU:CD   | 2.63                     | 0.41              |
| 1:F:217:ARG:CA   | 1:F:372:VAL:HG23 | 2.44                     | 0.41              |
| 1:F:233:ARG:HD2  | 1:F:351:GLU:OE2  | 2.21                     | 0.41              |
| 1:G:75:GLN:NE2   | 1:H:13:PRO:HG3   | 2.36                     | 0.41              |
| 1:G:502:LYS:HB3  | 1:G:502:LYS:HE3  | 1.90                     | 0.41              |
| 1:H:11:ILE:C     | 1:H:11:ILE:CD1   | 2.88                     | 0.41              |
| 1:H:29:ILE:CD1   | 1:H:112:GLU:HB2  | 2.50                     | 0.41              |
| 1:H:205:LYS:HZ3  | 1:H:358:GLU:HB2  | 1.86                     | 0.41              |
| 1:H:481:VAL:HG13 | 3:H:8528:ADP:C2  | 2.56                     | 0.41              |
| 1:C:17:GLN:CD    | 1:C:17:GLN:N     | 2.78                     | 0.41              |
| 1:C:109:ARG:HG2  | 1:C:109:ARG:NH1  | 2.36                     | 0.41              |
| 1:C:119:ILE:HD11 | 1:C:435:LEU:HD23 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:18:ARG:HA    | 1:D:521:VAL:O    | 2.21                     | 0.41              |
| 1:D:64:ASP:O     | 1:D:68:ILE:HG13  | 2.21                     | 0.41              |
| 1:D:172:GLU:OE1  | 1:D:172:GLU:CA   | 2.69                     | 0.41              |
| 1:D:294:GLN:HB2  | 1:D:321:MET:HE2  | 2.03                     | 0.41              |
| 1:F:216:VAL:O    | 1:F:372:VAL:HG23 | 2.20                     | 0.41              |
| 1:A:172:GLU:OE1  | 1:A:172:GLU:HA   | 2.22                     | 0.40              |
| 1:A:220:VAL:CG1  | 1:A:360:MET:HE2  | 2.51                     | 0.40              |
| 1:A:445:LYS:C    | 1:A:448:PRO:HD2  | 2.46                     | 0.40              |
| 1:B:35:ILE:HG22  | 1:B:36:ALA:N     | 2.35                     | 0.40              |
| 1:B:38:THR:O     | 1:B:50:LYS:CE    | 2.69                     | 0.40              |
| 1:B:166:ASN:O    | 1:B:168:GLU:N    | 2.54                     | 0.40              |
| 1:B:468:SER:O    | 1:B:471:LYS:N    | 2.54                     | 0.40              |
| 1:C:33:ARG:O     | 1:C:37:GLU:HG3   | 2.21                     | 0.40              |
| 1:D:348:GLU:O    | 1:D:349:VAL:CG2  | 2.67                     | 0.40              |
| 1:D:401:VAL:O    | 1:D:405:GLY:N    | 2.51                     | 0.40              |
| 1:E:232:LYS:HD3  | 1:E:232:LYS:HA   | 1.85                     | 0.40              |
| 1:E:253:THR:O    | 1:E:254:ASP:C    | 2.62                     | 0.40              |
| 1:F:13:PRO:HB2   | 1:F:16:THR:OG1   | 2.21                     | 0.40              |
| 1:F:300:LEU:HD23 | 1:F:300:LEU:HA   | 1.81                     | 0.40              |
| 1:G:136:GLN:HE21 | 1:G:136:GLN:CA   | 2.31                     | 0.40              |
| 1:H:76:HIS:HA    | 1:H:77:PRO:HD3   | 1.86                     | 0.40              |
| 1:H:85:VAL:HG13  | 1:H:507:SER:HB3  | 2.03                     | 0.40              |
| 1:H:196:ASP:OD1  | 1:H:198:ASP:HB2  | 2.21                     | 0.40              |
| 1:H:276:LEU:HD23 | 1:H:300:LEU:HB2  | 2.03                     | 0.40              |
| 1:H:359:ASN:C    | 1:H:360:MET:HG3  | 2.46                     | 0.40              |
| 1:B:423:ASP:O    | 1:B:426:ALA:HB3  | 2.20                     | 0.40              |
| 1:C:53:VAL:HG21  | 1:D:77:PRO:HG2   | 2.02                     | 0.40              |
| 1:C:195:VAL:HB   | 1:C:399:LYS:HG3  | 2.03                     | 0.40              |
| 1:D:370:LYS:HA   | 1:D:370:LYS:CE   | 2.46                     | 0.40              |
| 1:F:54:ASP:OD1   | 1:F:58:ASP:N     | 2.54                     | 0.40              |
| 1:F:380:THR:OG1  | 1:F:381:GLU:N    | 2.53                     | 0.40              |
| 1:G:204:LYS:HB2  | 1:G:204:LYS:HE3  | 1.90                     | 0.40              |
| 1:G:496:GLU:OE1  | 1:G:501:LYS:NZ   | 2.48                     | 0.40              |
| 1:H:469:GLU:CB   | 1:H:477:ILE:HG21 | 2.46                     | 0.40              |
| 1:A:106:GLU:HB2  | 1:A:446:ILE:HG12 | 2.03                     | 0.40              |
| 1:A:184:GLN:HA   | 1:A:184:GLN:HE21 | 1.87                     | 0.40              |
| 1:B:273:GLU:HG2  | 1:B:300:LEU:CD1  | 2.51                     | 0.40              |
| 1:B:466:VAL:CG2  | 1:B:486:PRO:HG3  | 2.42                     | 0.40              |
| 1:B:488:ASP:HB3  | 1:B:491:GLU:CG   | 2.48                     | 0.40              |
| 1:B:498:LEU:HD13 | 1:B:498:LEU:C    | 2.47                     | 0.40              |
| 1:C:73:ASP:O     | 1:D:13:PRO:HD3   | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:136:GLN:NE2  | 1:C:502:LYS:HG2  | 2.36                     | 0.40              |
| 1:C:469:GLU:HA   | 1:C:469:GLU:OE2  | 2.20                     | 0.40              |
| 1:D:475:LEU:HD12 | 1:D:475:LEU:O    | 2.21                     | 0.40              |
| 1:E:172:GLU:HA   | 1:E:172:GLU:OE1  | 2.21                     | 0.40              |
| 1:E:229:ARG:HG2  | 1:E:229:ARG:NH1  | 2.37                     | 0.40              |
| 1:F:14:GLU:C     | 1:F:16:THR:H     | 2.28                     | 0.40              |
| 1:F:443:ALA:C    | 1:F:445:LYS:H    | 2.29                     | 0.40              |
| 1:F:458:ASP:OD2  | 1:F:458:ASP:C    | 2.65                     | 0.40              |
| 1:F:525:LYS:O    | 1:F:526:ALA:HB2  | 2.22                     | 0.40              |
| 1:G:356:ALA:C    | 1:G:358:GLU:H    | 2.28                     | 0.40              |
| 1:H:35:ILE:HD13  | 1:H:35:ILE:HA    | 1.93                     | 0.40              |
| 1:A:490:LEU:HD12 | 1:A:490:LEU:HA   | 1.80                     | 0.40              |
| 1:B:145:ARG:NH1  | 1:B:145:ARG:CG   | 2.78                     | 0.40              |
| 1:C:304:TYR:O    | 1:C:308:TYR:CD1  | 2.75                     | 0.40              |
| 1:C:483:GLU:HA   | 1:C:483:GLU:OE1  | 2.21                     | 0.40              |
| 1:C:525:LYS:HD2  | 1:C:525:LYS:N    | 2.35                     | 0.40              |
| 1:D:227:HIS:HB3  | 1:D:230:MET:HG3  | 2.03                     | 0.40              |
| 1:D:229:ARG:HH12 | 1:E:332:ILE:H    | 1.69                     | 0.40              |
| 1:D:451:LEU:HD23 | 1:D:451:LEU:HA   | 1.97                     | 0.40              |
| 1:D:505:ILE:O    | 1:D:506:LYS:C    | 2.63                     | 0.40              |
| 1:E:18:ARG:HA    | 1:E:521:VAL:O    | 2.22                     | 0.40              |
| 1:E:225:VAL:CG1  | 1:E:230:MET:HB2  | 2.52                     | 0.40              |
| 1:G:458:ASP:O    | 1:G:459:THR:C    | 2.64                     | 0.40              |
| 1:H:76:HIS:HD2   | 1:H:78:ALA:HB3   | 1.84                     | 0.40              |
| 1:H:123:ILE:HG21 | 1:H:432:LYS:CB   | 2.45                     | 0.40              |
| 1:A:75:GLN:HG3   | 1:B:10:VAL:HG13  | 2.04                     | 0.40              |
| 1:A:227:HIS:HA   | 1:A:228:PRO:HD3  | 1.90                     | 0.40              |
| 1:B:418:LEU:O    | 1:B:422:LEU:HB2  | 2.22                     | 0.40              |
| 1:C:118:ASN:HD22 | 1:C:118:ASN:HA   | 1.57                     | 0.40              |
| 1:C:142:ILE:HB   | 1:C:475:LEU:HD21 | 2.01                     | 0.40              |
| 1:C:294:GLN:OE1  | 1:C:321:MET:HG3  | 2.21                     | 0.40              |
| 1:C:348:GLU:HB3  | 1:C:365:GLY:HA3  | 2.02                     | 0.40              |
| 1:C:416:ILE:HD13 | 1:C:466:VAL:HG12 | 2.03                     | 0.40              |
| 1:D:91:LYS:O     | 1:D:91:LYS:CG    | 2.70                     | 0.40              |
| 1:D:106:GLU:HG3  | 1:D:443:ALA:HB1  | 2.03                     | 0.40              |
| 1:D:106:GLU:HB2  | 1:D:446:ILE:HG12 | 2.03                     | 0.40              |
| 1:D:245:ALA:HB1  | 1:D:247:GLU:HG2  | 2.04                     | 0.40              |
| 1:D:257:ILE:HG22 | 1:D:259:ILE:HD12 | 2.04                     | 0.40              |
| 1:D:299:ASP:O    | 1:D:302:GLN:HB2  | 2.21                     | 0.40              |
| 1:E:26:ARG:CG    | 1:E:26:ARG:HH11  | 2.35                     | 0.40              |
| 1:E:143:ALA:HB3  | 1:E:145:ARG:HH12 | 1.87                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:184:GLN:HE21 | 1:E:184:GLN:CA   | 2.11                     | 0.40              |
| 1:H:147:ASP:OD2  | 1:H:148:PRO:HD2  | 2.20                     | 0.40              |
| 1:H:179:VAL:O    | 1:H:183:LYS:HG3  | 2.22                     | 0.40              |
| 1:H:409:PRO:HA   | 1:H:495:ILE:HG22 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 515/548 (94%)   | 468 (91%)  | 34 (7%)  | 13 (2%)  | 4           | 23 |
| 1   | B     | 515/548 (94%)   | 464 (90%)  | 41 (8%)  | 10 (2%)  | 6           | 30 |
| 1   | C     | 515/548 (94%)   | 463 (90%)  | 42 (8%)  | 10 (2%)  | 6           | 30 |
| 1   | D     | 515/548 (94%)   | 459 (89%)  | 46 (9%)  | 10 (2%)  | 6           | 30 |
| 1   | E     | 515/548 (94%)   | 468 (91%)  | 38 (7%)  | 9 (2%)   | 7           | 32 |
| 1   | F     | 515/548 (94%)   | 467 (91%)  | 36 (7%)  | 12 (2%)  | 5           | 25 |
| 1   | G     | 515/548 (94%)   | 452 (88%)  | 52 (10%) | 11 (2%)  | 5           | 27 |
| 1   | H     | 515/548 (94%)   | 459 (89%)  | 47 (9%)  | 9 (2%)   | 7           | 32 |
| All | All   | 4120/4384 (94%) | 3700 (90%) | 336 (8%) | 84 (2%)  | 6           | 28 |

All (84) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 148 | PRO  |
| 1   | A     | 367 | LYS  |
| 1   | B     | 167 | ALA  |
| 1   | B     | 248 | VAL  |
| 1   | C     | 148 | PRO  |
| 1   | C     | 167 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 148 | PRO  |
| 1   | D     | 367 | LYS  |
| 1   | E     | 150 | ASP  |
| 1   | E     | 248 | VAL  |
| 1   | E     | 367 | LYS  |
| 1   | F     | 148 | PRO  |
| 1   | F     | 367 | LYS  |
| 1   | G     | 11  | ILE  |
| 1   | G     | 148 | PRO  |
| 1   | H     | 367 | LYS  |
| 1   | A     | 236 | ASN  |
| 1   | A     | 473 | ARG  |
| 1   | A     | 475 | LEU  |
| 1   | B     | 367 | LYS  |
| 1   | C     | 152 | GLU  |
| 1   | C     | 235 | GLU  |
| 1   | C     | 367 | LYS  |
| 1   | C     | 430 | GLY  |
| 1   | D     | 167 | ALA  |
| 1   | D     | 248 | VAL  |
| 1   | E     | 47  | GLY  |
| 1   | E     | 148 | PRO  |
| 1   | E     | 168 | GLU  |
| 1   | E     | 235 | GLU  |
| 1   | F     | 168 | GLU  |
| 1   | F     | 236 | ASN  |
| 1   | F     | 459 | THR  |
| 1   | G     | 167 | ALA  |
| 1   | G     | 367 | LYS  |
| 1   | G     | 430 | GLY  |
| 1   | H     | 148 | PRO  |
| 1   | H     | 150 | ASP  |
| 1   | H     | 248 | VAL  |
| 1   | A     | 142 | ILE  |
| 1   | A     | 189 | LYS  |
| 1   | B     | 150 | ASP  |
| 1   | B     | 189 | LYS  |
| 1   | C     | 164 | GLY  |
| 1   | D     | 298 | ASP  |
| 1   | E     | 151 | GLU  |
| 1   | F     | 172 | GLU  |
| 1   | F     | 217 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 444 | LEU  |
| 1   | F     | 475 | LEU  |
| 1   | G     | 444 | LEU  |
| 1   | G     | 459 | THR  |
| 1   | H     | 164 | GLY  |
| 1   | H     | 235 | GLU  |
| 1   | H     | 475 | LEU  |
| 1   | A     | 167 | ALA  |
| 1   | B     | 459 | THR  |
| 1   | C     | 248 | VAL  |
| 1   | C     | 459 | THR  |
| 1   | D     | 58  | ASP  |
| 1   | D     | 235 | GLU  |
| 1   | F     | 235 | GLU  |
| 1   | F     | 248 | VAL  |
| 1   | G     | 152 | GLU  |
| 1   | G     | 427 | LYS  |
| 1   | H     | 13  | PRO  |
| 1   | A     | 164 | GLY  |
| 1   | A     | 248 | VAL  |
| 1   | B     | 172 | GLU  |
| 1   | B     | 298 | ASP  |
| 1   | B     | 444 | LEU  |
| 1   | C     | 166 | ASN  |
| 1   | D     | 150 | ASP  |
| 1   | D     | 164 | GLY  |
| 1   | H     | 217 | ARG  |
| 1   | A     | 150 | ASP  |
| 1   | D     | 157 | ILE  |
| 1   | F     | 164 | GLY  |
| 1   | G     | 248 | VAL  |
| 1   | A     | 94  | GLY  |
| 1   | A     | 210 | VAL  |
| 1   | E     | 430 | GLY  |
| 1   | G     | 349 | VAL  |
| 1   | B     | 148 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 422/441 (96%)   | 382 (90%)  | 40 (10%) | 8           | 31 |
| 1   | B     | 422/441 (96%)   | 388 (92%)  | 34 (8%)  | 11          | 38 |
| 1   | C     | 422/441 (96%)   | 385 (91%)  | 37 (9%)  | 9           | 35 |
| 1   | D     | 422/441 (96%)   | 385 (91%)  | 37 (9%)  | 9           | 35 |
| 1   | E     | 422/441 (96%)   | 384 (91%)  | 38 (9%)  | 9           | 34 |
| 1   | F     | 422/441 (96%)   | 386 (92%)  | 36 (8%)  | 10          | 36 |
| 1   | G     | 422/441 (96%)   | 392 (93%)  | 30 (7%)  | 13          | 43 |
| 1   | H     | 422/441 (96%)   | 393 (93%)  | 29 (7%)  | 14          | 45 |
| All | All   | 3376/3528 (96%) | 3095 (92%) | 281 (8%) | 10          | 37 |

All (281) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | GLU  |
| 1   | A     | 17  | GLN  |
| 1   | A     | 26  | ARG  |
| 1   | A     | 35  | ILE  |
| 1   | A     | 41  | THR  |
| 1   | A     | 54  | ASP  |
| 1   | A     | 59  | ILE  |
| 1   | A     | 91  | LYS  |
| 1   | A     | 110 | LYS  |
| 1   | A     | 126 | LYS  |
| 1   | A     | 148 | PRO  |
| 1   | A     | 155 | LEU  |
| 1   | A     | 168 | GLU  |
| 1   | A     | 171 | LYS  |
| 1   | A     | 190 | ASP  |
| 1   | A     | 212 | GLU  |
| 1   | A     | 214 | GLU  |
| 1   | A     | 222 | ASP  |
| 1   | A     | 241 | LEU  |
| 1   | A     | 246 | LEU  |
| 1   | A     | 262 | PRO  |
| 1   | A     | 276 | LEU  |
| 1   | A     | 298 | ASP  |
| 1   | A     | 315 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 336 | VAL  |
| 1   | A     | 358 | GLU  |
| 1   | A     | 369 | PRO  |
| 1   | A     | 370 | LYS  |
| 1   | A     | 381 | GLU  |
| 1   | A     | 415 | GLU  |
| 1   | A     | 421 | ARG  |
| 1   | A     | 424 | GLU  |
| 1   | A     | 446 | ILE  |
| 1   | A     | 449 | LYS  |
| 1   | A     | 466 | VAL  |
| 1   | A     | 483 | GLU  |
| 1   | A     | 490 | LEU  |
| 1   | A     | 498 | LEU  |
| 1   | A     | 501 | LYS  |
| 1   | A     | 525 | LYS  |
| 1   | B     | 11  | ILE  |
| 1   | B     | 17  | GLN  |
| 1   | B     | 20  | VAL  |
| 1   | B     | 23  | ASP  |
| 1   | B     | 26  | ARG  |
| 1   | B     | 35  | ILE  |
| 1   | B     | 41  | THR  |
| 1   | B     | 54  | ASP  |
| 1   | B     | 59  | ILE  |
| 1   | B     | 91  | LYS  |
| 1   | B     | 110 | LYS  |
| 1   | B     | 126 | LYS  |
| 1   | B     | 133 | GLU  |
| 1   | B     | 170 | HIS  |
| 1   | B     | 171 | LYS  |
| 1   | B     | 190 | ASP  |
| 1   | B     | 222 | ASP  |
| 1   | B     | 241 | LEU  |
| 1   | B     | 276 | LEU  |
| 1   | B     | 298 | ASP  |
| 1   | B     | 315 | ARG  |
| 1   | B     | 336 | VAL  |
| 1   | B     | 370 | LYS  |
| 1   | B     | 415 | GLU  |
| 1   | B     | 421 | ARG  |
| 1   | B     | 435 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 446 | ILE  |
| 1   | B     | 449 | LYS  |
| 1   | B     | 462 | MET  |
| 1   | B     | 468 | SER  |
| 1   | B     | 483 | GLU  |
| 1   | B     | 498 | LEU  |
| 1   | B     | 519 | ASP  |
| 1   | B     | 525 | LYS  |
| 1   | C     | 11  | ILE  |
| 1   | C     | 14  | GLU  |
| 1   | C     | 17  | GLN  |
| 1   | C     | 26  | ARG  |
| 1   | C     | 35  | ILE  |
| 1   | C     | 41  | THR  |
| 1   | C     | 54  | ASP  |
| 1   | C     | 91  | LYS  |
| 1   | C     | 107 | LEU  |
| 1   | C     | 110 | LYS  |
| 1   | C     | 118 | ASN  |
| 1   | C     | 126 | LYS  |
| 1   | C     | 148 | PRO  |
| 1   | C     | 170 | HIS  |
| 1   | C     | 171 | LYS  |
| 1   | C     | 190 | ASP  |
| 1   | C     | 214 | GLU  |
| 1   | C     | 222 | ASP  |
| 1   | C     | 224 | GLU  |
| 1   | C     | 241 | LEU  |
| 1   | C     | 247 | GLU  |
| 1   | C     | 252 | GLU  |
| 1   | C     | 276 | LEU  |
| 1   | C     | 298 | ASP  |
| 1   | C     | 315 | ARG  |
| 1   | C     | 358 | GLU  |
| 1   | C     | 370 | LYS  |
| 1   | C     | 381 | GLU  |
| 1   | C     | 415 | GLU  |
| 1   | C     | 421 | ARG  |
| 1   | C     | 428 | GLN  |
| 1   | C     | 435 | LEU  |
| 1   | C     | 446 | ILE  |
| 1   | C     | 449 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 483 | GLU  |
| 1   | C     | 498 | LEU  |
| 1   | C     | 525 | LYS  |
| 1   | D     | 11  | ILE  |
| 1   | D     | 17  | GLN  |
| 1   | D     | 26  | ARG  |
| 1   | D     | 35  | ILE  |
| 1   | D     | 63  | ASN  |
| 1   | D     | 91  | LYS  |
| 1   | D     | 107 | LEU  |
| 1   | D     | 110 | LYS  |
| 1   | D     | 126 | LYS  |
| 1   | D     | 148 | PRO  |
| 1   | D     | 154 | LEU  |
| 1   | D     | 171 | LYS  |
| 1   | D     | 190 | ASP  |
| 1   | D     | 212 | GLU  |
| 1   | D     | 222 | ASP  |
| 1   | D     | 241 | LEU  |
| 1   | D     | 252 | GLU  |
| 1   | D     | 258 | ASN  |
| 1   | D     | 276 | LEU  |
| 1   | D     | 282 | HIS  |
| 1   | D     | 289 | ASN  |
| 1   | D     | 298 | ASP  |
| 1   | D     | 315 | ARG  |
| 1   | D     | 336 | VAL  |
| 1   | D     | 358 | GLU  |
| 1   | D     | 364 | GLU  |
| 1   | D     | 370 | LYS  |
| 1   | D     | 415 | GLU  |
| 1   | D     | 421 | ARG  |
| 1   | D     | 428 | GLN  |
| 1   | D     | 446 | ILE  |
| 1   | D     | 449 | LYS  |
| 1   | D     | 483 | GLU  |
| 1   | D     | 490 | LEU  |
| 1   | D     | 498 | LEU  |
| 1   | D     | 501 | LYS  |
| 1   | D     | 519 | ASP  |
| 1   | E     | 11  | ILE  |
| 1   | E     | 14  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 17  | GLN  |
| 1   | E     | 23  | ASP  |
| 1   | E     | 26  | ARG  |
| 1   | E     | 35  | ILE  |
| 1   | E     | 41  | THR  |
| 1   | E     | 48  | MET  |
| 1   | E     | 59  | ILE  |
| 1   | E     | 72  | ILE  |
| 1   | E     | 80  | LYS  |
| 1   | E     | 91  | LYS  |
| 1   | E     | 110 | LYS  |
| 1   | E     | 126 | LYS  |
| 1   | E     | 148 | PRO  |
| 1   | E     | 154 | LEU  |
| 1   | E     | 163 | THR  |
| 1   | E     | 214 | GLU  |
| 1   | E     | 222 | ASP  |
| 1   | E     | 241 | LEU  |
| 1   | E     | 246 | LEU  |
| 1   | E     | 251 | THR  |
| 1   | E     | 276 | LEU  |
| 1   | E     | 286 | THR  |
| 1   | E     | 291 | VAL  |
| 1   | E     | 293 | VAL  |
| 1   | E     | 298 | ASP  |
| 1   | E     | 364 | GLU  |
| 1   | E     | 370 | LYS  |
| 1   | E     | 415 | GLU  |
| 1   | E     | 421 | ARG  |
| 1   | E     | 446 | ILE  |
| 1   | E     | 449 | LYS  |
| 1   | E     | 462 | MET  |
| 1   | E     | 483 | GLU  |
| 1   | E     | 498 | LEU  |
| 1   | E     | 501 | LYS  |
| 1   | E     | 519 | ASP  |
| 1   | F     | 11  | ILE  |
| 1   | F     | 17  | GLN  |
| 1   | F     | 23  | ASP  |
| 1   | F     | 26  | ARG  |
| 1   | F     | 35  | ILE  |
| 1   | F     | 41  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 63  | ASN  |
| 1   | F     | 91  | LYS  |
| 1   | F     | 110 | LYS  |
| 1   | F     | 118 | ASN  |
| 1   | F     | 126 | LYS  |
| 1   | F     | 128 | TYR  |
| 1   | F     | 133 | GLU  |
| 1   | F     | 148 | PRO  |
| 1   | F     | 154 | LEU  |
| 1   | F     | 171 | LYS  |
| 1   | F     | 190 | ASP  |
| 1   | F     | 222 | ASP  |
| 1   | F     | 241 | LEU  |
| 1   | F     | 246 | LEU  |
| 1   | F     | 276 | LEU  |
| 1   | F     | 298 | ASP  |
| 1   | F     | 315 | ARG  |
| 1   | F     | 336 | VAL  |
| 1   | F     | 338 | ASP  |
| 1   | F     | 370 | LYS  |
| 1   | F     | 381 | GLU  |
| 1   | F     | 415 | GLU  |
| 1   | F     | 421 | ARG  |
| 1   | F     | 446 | ILE  |
| 1   | F     | 449 | LYS  |
| 1   | F     | 462 | MET  |
| 1   | F     | 483 | GLU  |
| 1   | F     | 490 | LEU  |
| 1   | F     | 498 | LEU  |
| 1   | F     | 501 | LYS  |
| 1   | G     | 11  | ILE  |
| 1   | G     | 17  | GLN  |
| 1   | G     | 26  | ARG  |
| 1   | G     | 91  | LYS  |
| 1   | G     | 110 | LYS  |
| 1   | G     | 118 | ASN  |
| 1   | G     | 126 | LYS  |
| 1   | G     | 128 | TYR  |
| 1   | G     | 148 | PRO  |
| 1   | G     | 154 | LEU  |
| 1   | G     | 171 | LYS  |
| 1   | G     | 190 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 222 | ASP  |
| 1   | G     | 224 | GLU  |
| 1   | G     | 241 | LEU  |
| 1   | G     | 246 | LEU  |
| 1   | G     | 260 | THR  |
| 1   | G     | 276 | LEU  |
| 1   | G     | 298 | ASP  |
| 1   | G     | 315 | ARG  |
| 1   | G     | 336 | VAL  |
| 1   | G     | 370 | LYS  |
| 1   | G     | 395 | VAL  |
| 1   | G     | 415 | GLU  |
| 1   | G     | 421 | ARG  |
| 1   | G     | 446 | ILE  |
| 1   | G     | 449 | LYS  |
| 1   | G     | 498 | LEU  |
| 1   | G     | 501 | LYS  |
| 1   | G     | 525 | LYS  |
| 1   | H     | 11  | ILE  |
| 1   | H     | 17  | GLN  |
| 1   | H     | 26  | ARG  |
| 1   | H     | 35  | ILE  |
| 1   | H     | 54  | ASP  |
| 1   | H     | 91  | LYS  |
| 1   | H     | 107 | LEU  |
| 1   | H     | 126 | LYS  |
| 1   | H     | 148 | PRO  |
| 1   | H     | 171 | LYS  |
| 1   | H     | 190 | ASP  |
| 1   | H     | 222 | ASP  |
| 1   | H     | 241 | LEU  |
| 1   | H     | 246 | LEU  |
| 1   | H     | 262 | PRO  |
| 1   | H     | 276 | LEU  |
| 1   | H     | 298 | ASP  |
| 1   | H     | 338 | ASP  |
| 1   | H     | 370 | LYS  |
| 1   | H     | 381 | GLU  |
| 1   | H     | 415 | GLU  |
| 1   | H     | 421 | ARG  |
| 1   | H     | 446 | ILE  |
| 1   | H     | 449 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 483 | GLU  |
| 1   | H     | 490 | LEU  |
| 1   | H     | 498 | LEU  |
| 1   | H     | 501 | LYS  |
| 1   | H     | 519 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | GLN  |
| 1   | A     | 28  | ASN  |
| 1   | A     | 75  | GLN  |
| 1   | A     | 76  | HIS  |
| 1   | A     | 117 | GLN  |
| 1   | A     | 118 | ASN  |
| 1   | A     | 136 | GLN  |
| 1   | A     | 166 | ASN  |
| 1   | A     | 184 | GLN  |
| 1   | A     | 258 | ASN  |
| 1   | A     | 264 | GLN  |
| 1   | A     | 271 | GLN  |
| 1   | A     | 282 | HIS  |
| 1   | A     | 285 | GLN  |
| 1   | A     | 294 | GLN  |
| 1   | A     | 439 | ASN  |
| 1   | A     | 503 | GLN  |
| 1   | B     | 17  | GLN  |
| 1   | B     | 28  | ASN  |
| 1   | B     | 76  | HIS  |
| 1   | B     | 118 | ASN  |
| 1   | B     | 136 | GLN  |
| 1   | B     | 166 | ASN  |
| 1   | B     | 170 | HIS  |
| 1   | B     | 184 | GLN  |
| 1   | B     | 258 | ASN  |
| 1   | B     | 264 | GLN  |
| 1   | B     | 282 | HIS  |
| 1   | B     | 285 | GLN  |
| 1   | B     | 503 | GLN  |
| 1   | C     | 17  | GLN  |
| 1   | C     | 28  | ASN  |
| 1   | C     | 75  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 76  | HIS  |
| 1   | C     | 118 | ASN  |
| 1   | C     | 136 | GLN  |
| 1   | C     | 166 | ASN  |
| 1   | C     | 184 | GLN  |
| 1   | C     | 258 | ASN  |
| 1   | C     | 264 | GLN  |
| 1   | C     | 285 | GLN  |
| 1   | C     | 368 | ASN  |
| 1   | D     | 17  | GLN  |
| 1   | D     | 28  | ASN  |
| 1   | D     | 76  | HIS  |
| 1   | D     | 118 | ASN  |
| 1   | D     | 136 | GLN  |
| 1   | D     | 170 | HIS  |
| 1   | D     | 184 | GLN  |
| 1   | D     | 236 | ASN  |
| 1   | D     | 258 | ASN  |
| 1   | D     | 264 | GLN  |
| 1   | D     | 285 | GLN  |
| 1   | D     | 439 | ASN  |
| 1   | D     | 503 | GLN  |
| 1   | E     | 17  | GLN  |
| 1   | E     | 28  | ASN  |
| 1   | E     | 76  | HIS  |
| 1   | E     | 118 | ASN  |
| 1   | E     | 136 | GLN  |
| 1   | E     | 166 | ASN  |
| 1   | E     | 258 | ASN  |
| 1   | E     | 264 | GLN  |
| 1   | E     | 285 | GLN  |
| 1   | E     | 335 | ASN  |
| 1   | E     | 359 | ASN  |
| 1   | E     | 382 | HIS  |
| 1   | E     | 439 | ASN  |
| 1   | F     | 17  | GLN  |
| 1   | F     | 28  | ASN  |
| 1   | F     | 75  | GLN  |
| 1   | F     | 76  | HIS  |
| 1   | F     | 118 | ASN  |
| 1   | F     | 136 | GLN  |
| 1   | F     | 166 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 170 | HIS  |
| 1   | F     | 184 | GLN  |
| 1   | F     | 236 | ASN  |
| 1   | F     | 258 | ASN  |
| 1   | F     | 264 | GLN  |
| 1   | F     | 282 | HIS  |
| 1   | F     | 285 | GLN  |
| 1   | F     | 303 | HIS  |
| 1   | F     | 503 | GLN  |
| 1   | G     | 17  | GLN  |
| 1   | G     | 28  | ASN  |
| 1   | G     | 63  | ASN  |
| 1   | G     | 76  | HIS  |
| 1   | G     | 118 | ASN  |
| 1   | G     | 136 | GLN  |
| 1   | G     | 166 | ASN  |
| 1   | G     | 184 | GLN  |
| 1   | G     | 258 | ASN  |
| 1   | G     | 264 | GLN  |
| 1   | G     | 285 | GLN  |
| 1   | G     | 368 | ASN  |
| 1   | G     | 503 | GLN  |
| 1   | H     | 17  | GLN  |
| 1   | H     | 25  | GLN  |
| 1   | H     | 28  | ASN  |
| 1   | H     | 76  | HIS  |
| 1   | H     | 118 | ASN  |
| 1   | H     | 136 | GLN  |
| 1   | H     | 166 | ASN  |
| 1   | H     | 170 | HIS  |
| 1   | H     | 184 | GLN  |
| 1   | H     | 258 | ASN  |
| 1   | H     | 264 | GLN  |
| 1   | H     | 282 | HIS  |
| 1   | H     | 285 | GLN  |
| 1   | H     | 439 | ASN  |
| 1   | H     | 503 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ADP  | D     | 4528 | 2    | 28,29,29     | 1.76 | 7 (25%)  | 43,45,45    | 2.11 | 10 (23%) |
| 3   | ADP  | C     | 3528 | 2    | 28,29,29     | 1.71 | 7 (25%)  | 43,45,45    | 2.10 | 10 (23%) |
| 3   | ADP  | H     | 8528 | 2    | 28,29,29     | 1.68 | 7 (25%)  | 43,45,45    | 2.10 | 10 (23%) |
| 3   | ADP  | A     | 1528 | 2    | 28,29,29     | 1.77 | 7 (25%)  | 43,45,45    | 2.04 | 10 (23%) |
| 3   | ADP  | E     | 5528 | 2    | 28,29,29     | 1.72 | 7 (25%)  | 43,45,45    | 2.04 | 10 (23%) |
| 3   | ADP  | B     | 2528 | 2    | 28,29,29     | 1.69 | 7 (25%)  | 43,45,45    | 2.05 | 9 (20%)  |
| 3   | ADP  | F     | 6528 | -    | 28,29,29     | 1.76 | 7 (25%)  | 43,45,45    | 2.06 | 9 (20%)  |
| 3   | ADP  | G     | 7528 | 2    | 28,29,29     | 1.69 | 7 (25%)  | 43,45,45    | 2.06 | 10 (23%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | ADP  | D     | 4528 | 2    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | ADP  | C     | 3528 | 2    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | ADP  | H     | 8528 | 2    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | ADP  | A     | 1528 | 2    | -       | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | ADP  | E     | 5528 | 2    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | ADP  | B     | 2528 | 2    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | ADP  | F     | 6528 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | ADP  | G     | 7528 | 2    | -       | 2/16/32/32 | 0/3/3/3 |

All (56) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | F     | 6528 | ADP  | C5-N7  | -4.33 | 1.31        | 1.39     |
| 3   | A     | 1528 | ADP  | C5-N7  | -4.28 | 1.31        | 1.39     |
| 3   | H     | 8528 | ADP  | C5-N7  | -4.12 | 1.31        | 1.39     |
| 3   | B     | 2528 | ADP  | C5-N7  | -4.08 | 1.31        | 1.39     |
| 3   | G     | 7528 | ADP  | C5-N7  | -3.72 | 1.32        | 1.39     |
| 3   | C     | 3528 | ADP  | C5-N7  | -3.71 | 1.32        | 1.39     |
| 3   | D     | 4528 | ADP  | PB-O3B | 3.60  | 1.68        | 1.54     |
| 3   | E     | 5528 | ADP  | C5-N7  | -3.52 | 1.32        | 1.39     |
| 3   | H     | 8528 | ADP  | PB-O3B | 3.45  | 1.67        | 1.54     |
| 3   | D     | 4528 | ADP  | C5-N7  | -3.45 | 1.32        | 1.39     |
| 3   | E     | 5528 | ADP  | PB-O3B | 3.44  | 1.67        | 1.54     |
| 3   | G     | 7528 | ADP  | C4-N9  | -3.43 | 1.30        | 1.37     |
| 3   | C     | 3528 | ADP  | PB-O3B | 3.38  | 1.67        | 1.54     |
| 3   | A     | 1528 | ADP  | PB-O3B | 3.38  | 1.67        | 1.54     |
| 3   | F     | 6528 | ADP  | PB-O3B | 3.37  | 1.67        | 1.54     |
| 3   | A     | 1528 | ADP  | C4-N9  | -3.34 | 1.30        | 1.37     |
| 3   | B     | 2528 | ADP  | C4-N9  | -3.22 | 1.31        | 1.37     |
| 3   | B     | 2528 | ADP  | PB-O3B | 3.16  | 1.66        | 1.54     |
| 3   | E     | 5528 | ADP  | C4-N9  | -3.12 | 1.31        | 1.37     |
| 3   | C     | 3528 | ADP  | C4-N9  | -3.02 | 1.31        | 1.37     |
| 3   | D     | 4528 | ADP  | C4-N3  | 2.95  | 1.39        | 1.34     |
| 3   | G     | 7528 | ADP  | PB-O3B | 2.93  | 1.65        | 1.54     |
| 3   | D     | 4528 | ADP  | C5-C4  | 2.84  | 1.44        | 1.39     |
| 3   | H     | 8528 | ADP  | C4-N9  | -2.83 | 1.31        | 1.37     |
| 3   | E     | 5528 | ADP  | C5-C4  | 2.83  | 1.44        | 1.39     |
| 3   | G     | 7528 | ADP  | C5-C4  | 2.79  | 1.44        | 1.39     |
| 3   | F     | 6528 | ADP  | C5-C4  | 2.79  | 1.44        | 1.39     |
| 3   | A     | 1528 | ADP  | C5-C4  | 2.74  | 1.44        | 1.39     |
| 3   | B     | 2528 | ADP  | C5-C4  | 2.74  | 1.44        | 1.39     |
| 3   | F     | 6528 | ADP  | C4-N9  | -2.72 | 1.32        | 1.37     |
| 3   | C     | 3528 | ADP  | C5-C4  | 2.70  | 1.43        | 1.39     |
| 3   | D     | 4528 | ADP  | C4-N9  | -2.70 | 1.32        | 1.37     |
| 3   | D     | 4528 | ADP  | C2-N1  | 2.65  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | G     | 7528 | ADP  | C2-N1 | 2.64 | 1.38        | 1.33     |
| 3   | A     | 1528 | ADP  | C2-N1 | 2.63 | 1.38        | 1.33     |
| 3   | H     | 8528 | ADP  | C5-C4 | 2.62 | 1.43        | 1.39     |
| 3   | F     | 6528 | ADP  | C2-N3 | 2.57 | 1.38        | 1.33     |
| 3   | C     | 3528 | ADP  | C2-N3 | 2.57 | 1.38        | 1.33     |
| 3   | G     | 7528 | ADP  | C2-N3 | 2.56 | 1.38        | 1.33     |
| 3   | D     | 4528 | ADP  | C2-N3 | 2.50 | 1.38        | 1.33     |
| 3   | F     | 6528 | ADP  | C2-N1 | 2.47 | 1.38        | 1.33     |
| 3   | B     | 2528 | ADP  | C2-N1 | 2.45 | 1.38        | 1.33     |
| 3   | E     | 5528 | ADP  | C2-N1 | 2.44 | 1.38        | 1.33     |
| 3   | F     | 6528 | ADP  | C4-N3 | 2.43 | 1.39        | 1.34     |
| 3   | A     | 1528 | ADP  | C2-N3 | 2.40 | 1.38        | 1.33     |
| 3   | H     | 8528 | ADP  | C2-N1 | 2.40 | 1.38        | 1.33     |
| 3   | E     | 5528 | ADP  | C4-N3 | 2.35 | 1.38        | 1.34     |
| 3   | A     | 1528 | ADP  | C4-N3 | 2.34 | 1.38        | 1.34     |
| 3   | H     | 8528 | ADP  | C2-N3 | 2.34 | 1.38        | 1.33     |
| 3   | B     | 2528 | ADP  | C4-N3 | 2.34 | 1.38        | 1.34     |
| 3   | H     | 8528 | ADP  | C4-N3 | 2.32 | 1.38        | 1.34     |
| 3   | G     | 7528 | ADP  | C4-N3 | 2.32 | 1.38        | 1.34     |
| 3   | C     | 3528 | ADP  | C2-N1 | 2.32 | 1.38        | 1.33     |
| 3   | C     | 3528 | ADP  | C4-N3 | 2.18 | 1.38        | 1.34     |
| 3   | B     | 2528 | ADP  | C2-N3 | 2.18 | 1.37        | 1.33     |
| 3   | E     | 5528 | ADP  | C2-N3 | 2.09 | 1.37        | 1.33     |

All (78) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | H     | 8528 | ADP  | N3-C2-N1 | -6.76 | 118.35      | 128.58   |
| 3   | D     | 4528 | ADP  | N3-C2-N1 | -6.74 | 118.37      | 128.58   |
| 3   | A     | 1528 | ADP  | N3-C2-N1 | -6.69 | 118.45      | 128.58   |
| 3   | G     | 7528 | ADP  | N3-C2-N1 | -6.69 | 118.46      | 128.58   |
| 3   | B     | 2528 | ADP  | N3-C2-N1 | -6.68 | 118.46      | 128.58   |
| 3   | F     | 6528 | ADP  | N3-C2-N1 | -6.65 | 118.51      | 128.58   |
| 3   | C     | 3528 | ADP  | N3-C2-N1 | -6.64 | 118.53      | 128.58   |
| 3   | E     | 5528 | ADP  | N3-C2-N1 | -6.57 | 118.64      | 128.58   |
| 3   | F     | 6528 | ADP  | C5-C4-N3 | -5.22 | 119.53      | 126.72   |
| 3   | H     | 8528 | ADP  | C5-C4-N3 | -5.03 | 119.78      | 126.72   |
| 3   | C     | 3528 | ADP  | C5-C4-N3 | -4.99 | 119.84      | 126.72   |
| 3   | D     | 4528 | ADP  | C5-C4-N3 | -4.94 | 119.92      | 126.72   |
| 3   | B     | 2528 | ADP  | C5-C4-N3 | -4.85 | 120.04      | 126.72   |
| 3   | E     | 5528 | ADP  | C5-C4-N3 | -4.81 | 120.09      | 126.72   |
| 3   | A     | 1528 | ADP  | C5-C4-N3 | -4.78 | 120.13      | 126.72   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | G     | 7528 | ADP  | C5-C4-N3   | -4.77 | 120.15      | 126.72   |
| 3   | D     | 4528 | ADP  | C2-N3-C4   | 4.58  | 123.03      | 111.83   |
| 3   | F     | 6528 | ADP  | C2-N3-C4   | 4.55  | 122.95      | 111.83   |
| 3   | C     | 3528 | ADP  | C2-N3-C4   | 4.54  | 122.91      | 111.83   |
| 3   | H     | 8528 | ADP  | C2-N3-C4   | 4.49  | 122.81      | 111.83   |
| 3   | E     | 5528 | ADP  | C2-N3-C4   | 4.46  | 122.72      | 111.83   |
| 3   | B     | 2528 | ADP  | C2-N3-C4   | 4.45  | 122.70      | 111.83   |
| 3   | G     | 7528 | ADP  | C2-N3-C4   | 4.42  | 122.62      | 111.83   |
| 3   | A     | 1528 | ADP  | C2-N3-C4   | 4.37  | 122.50      | 111.83   |
| 3   | E     | 5528 | ADP  | C4-C5-N7   | -3.90 | 106.12      | 110.58   |
| 3   | C     | 3528 | ADP  | C4-C5-N7   | -3.88 | 106.14      | 110.58   |
| 3   | D     | 4528 | ADP  | C4-C5-N7   | -3.86 | 106.17      | 110.58   |
| 3   | F     | 6528 | ADP  | N3-C4-N9   | 3.81  | 133.64      | 127.17   |
| 3   | D     | 4528 | ADP  | C5-N7-C8   | 3.74  | 109.33      | 103.45   |
| 3   | H     | 8528 | ADP  | C5-N7-C8   | 3.74  | 109.33      | 103.45   |
| 3   | G     | 7528 | ADP  | N9-C8-N7   | -3.74 | 108.63      | 113.94   |
| 3   | G     | 7528 | ADP  | C4-C5-N7   | -3.72 | 106.33      | 110.58   |
| 3   | C     | 3528 | ADP  | N9-C8-N7   | -3.70 | 108.68      | 113.94   |
| 3   | D     | 4528 | ADP  | N9-C8-N7   | -3.70 | 108.69      | 113.94   |
| 3   | E     | 5528 | ADP  | N9-C8-N7   | -3.70 | 108.69      | 113.94   |
| 3   | H     | 8528 | ADP  | C4-C5-N7   | -3.69 | 106.36      | 110.58   |
| 3   | F     | 6528 | ADP  | C4-C5-N7   | -3.69 | 106.37      | 110.58   |
| 3   | B     | 2528 | ADP  | C4-C5-N7   | -3.64 | 106.42      | 110.58   |
| 3   | F     | 6528 | ADP  | C5-N7-C8   | 3.63  | 109.16      | 103.45   |
| 3   | A     | 1528 | ADP  | C4-C5-N7   | -3.62 | 106.44      | 110.58   |
| 3   | H     | 8528 | ADP  | N9-C8-N7   | -3.61 | 108.81      | 113.94   |
| 3   | H     | 8528 | ADP  | N3-C4-N9   | 3.61  | 133.31      | 127.17   |
| 3   | E     | 5528 | ADP  | C5-N7-C8   | 3.61  | 109.12      | 103.45   |
| 3   | C     | 3528 | ADP  | C5-N7-C8   | 3.59  | 109.09      | 103.45   |
| 3   | A     | 1528 | ADP  | C5-N7-C8   | 3.57  | 109.05      | 103.45   |
| 3   | B     | 2528 | ADP  | N9-C8-N7   | -3.55 | 108.90      | 113.94   |
| 3   | A     | 1528 | ADP  | N9-C8-N7   | -3.55 | 108.91      | 113.94   |
| 3   | B     | 2528 | ADP  | C5-N7-C8   | 3.52  | 108.98      | 103.45   |
| 3   | D     | 4528 | ADP  | N3-C4-N9   | 3.52  | 133.15      | 127.17   |
| 3   | A     | 1528 | ADP  | N3-C4-N9   | 3.51  | 133.13      | 127.17   |
| 3   | G     | 7528 | ADP  | C5-N7-C8   | 3.47  | 108.90      | 103.45   |
| 3   | C     | 3528 | ADP  | N3-C4-N9   | 3.45  | 133.03      | 127.17   |
| 3   | B     | 2528 | ADP  | N3-C4-N9   | 3.42  | 132.98      | 127.17   |
| 3   | E     | 5528 | ADP  | N3-C4-N9   | 3.35  | 132.87      | 127.17   |
| 3   | G     | 7528 | ADP  | N3-C4-N9   | 3.30  | 132.78      | 127.17   |
| 3   | F     | 6528 | ADP  | N9-C8-N7   | -3.25 | 109.33      | 113.94   |
| 3   | H     | 8528 | ADP  | O4'-C1'-N9 | 3.20  | 114.24      | 108.09   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 3   | G     | 7528 | ADP  | C4-N9-C8   | 3.16 | 109.06      | 105.74   |
| 3   | E     | 5528 | ADP  | C4-N9-C8   | 3.14 | 109.03      | 105.74   |
| 3   | C     | 3528 | ADP  | C4-N9-C8   | 3.06 | 108.95      | 105.74   |
| 3   | D     | 4528 | ADP  | C4-N9-C8   | 2.98 | 108.87      | 105.74   |
| 3   | A     | 1528 | ADP  | C4-N9-C8   | 2.97 | 108.86      | 105.74   |
| 3   | B     | 2528 | ADP  | C4-N9-C8   | 2.84 | 108.72      | 105.74   |
| 3   | H     | 8528 | ADP  | C4-N9-C8   | 2.72 | 108.59      | 105.74   |
| 3   | D     | 4528 | ADP  | C6-C5-N7   | 2.68 | 137.26      | 132.09   |
| 3   | E     | 5528 | ADP  | C6-C5-N7   | 2.68 | 137.26      | 132.09   |
| 3   | G     | 7528 | ADP  | O4'-C1'-N9 | 2.63 | 113.14      | 108.09   |
| 3   | C     | 3528 | ADP  | C6-C5-N7   | 2.60 | 137.11      | 132.09   |
| 3   | C     | 3528 | ADP  | O4'-C1'-N9 | 2.55 | 112.99      | 108.09   |
| 3   | B     | 2528 | ADP  | C6-C5-N7   | 2.54 | 136.99      | 132.09   |
| 3   | G     | 7528 | ADP  | C6-C5-N7   | 2.53 | 136.97      | 132.09   |
| 3   | F     | 6528 | ADP  | C4-N9-C8   | 2.45 | 108.31      | 105.74   |
| 3   | H     | 8528 | ADP  | C6-C5-N7   | 2.39 | 136.71      | 132.09   |
| 3   | A     | 1528 | ADP  | C6-C5-N7   | 2.34 | 136.61      | 132.09   |
| 3   | F     | 6528 | ADP  | C6-C5-N7   | 2.32 | 136.56      | 132.09   |
| 3   | D     | 4528 | ADP  | O4'-C1'-N9 | 2.07 | 112.07      | 108.09   |
| 3   | A     | 1528 | ADP  | O4'-C1'-N9 | 2.03 | 111.98      | 108.09   |
| 3   | E     | 5528 | ADP  | C2-N1-C6   | 2.02 | 122.04      | 118.73   |

There are no chirality outliers.

All (16) torsion outliers are listed below:

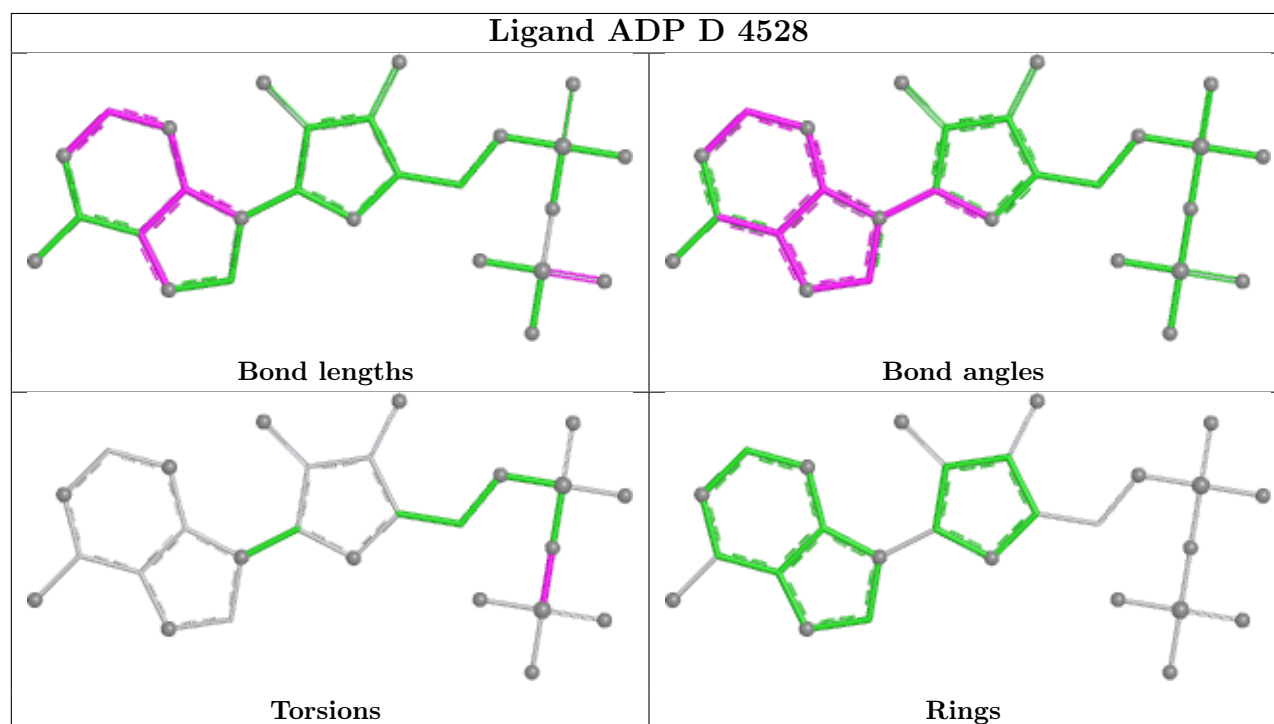
| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 3   | A     | 1528 | ADP  | PA-O3A-PB-O3B |
| 3   | B     | 2528 | ADP  | PA-O3A-PB-O3B |
| 3   | C     | 3528 | ADP  | PA-O3A-PB-O3B |
| 3   | D     | 4528 | ADP  | PA-O3A-PB-O3B |
| 3   | E     | 5528 | ADP  | PA-O3A-PB-O3B |
| 3   | F     | 6528 | ADP  | PA-O3A-PB-O3B |
| 3   | G     | 7528 | ADP  | PA-O3A-PB-O3B |
| 3   | H     | 8528 | ADP  | PA-O3A-PB-O3B |
| 3   | A     | 1528 | ADP  | PA-O3A-PB-O2B |
| 3   | B     | 2528 | ADP  | PA-O3A-PB-O2B |
| 3   | C     | 3528 | ADP  | PA-O3A-PB-O2B |
| 3   | D     | 4528 | ADP  | PA-O3A-PB-O2B |
| 3   | E     | 5528 | ADP  | PA-O3A-PB-O2B |
| 3   | F     | 6528 | ADP  | PA-O3A-PB-O2B |
| 3   | G     | 7528 | ADP  | PA-O3A-PB-O2B |
| 3   | H     | 8528 | ADP  | PA-O3A-PB-O2B |

There are no ring outliers.

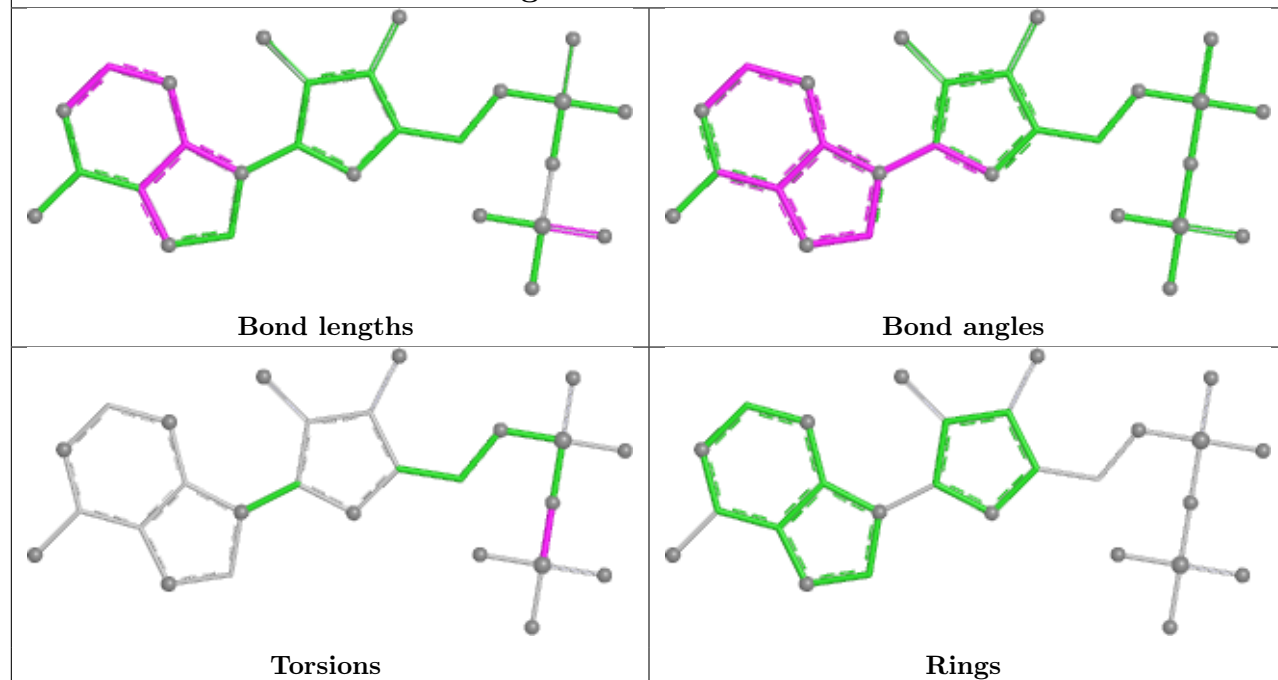
4 monomers are involved in 5 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | H     | 8528 | ADP  | 1       | 0            |
| 3   | B     | 2528 | ADP  | 1       | 0            |
| 3   | F     | 6528 | ADP  | 1       | 0            |
| 3   | G     | 7528 | ADP  | 2       | 0            |

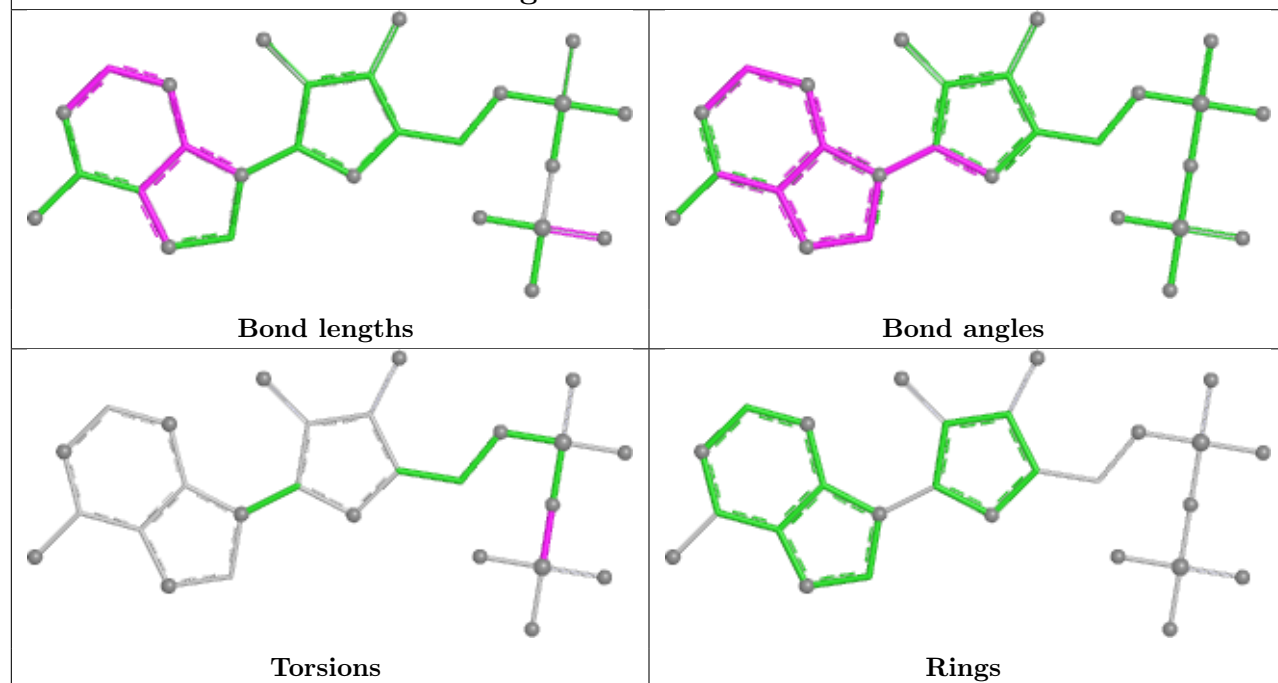
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



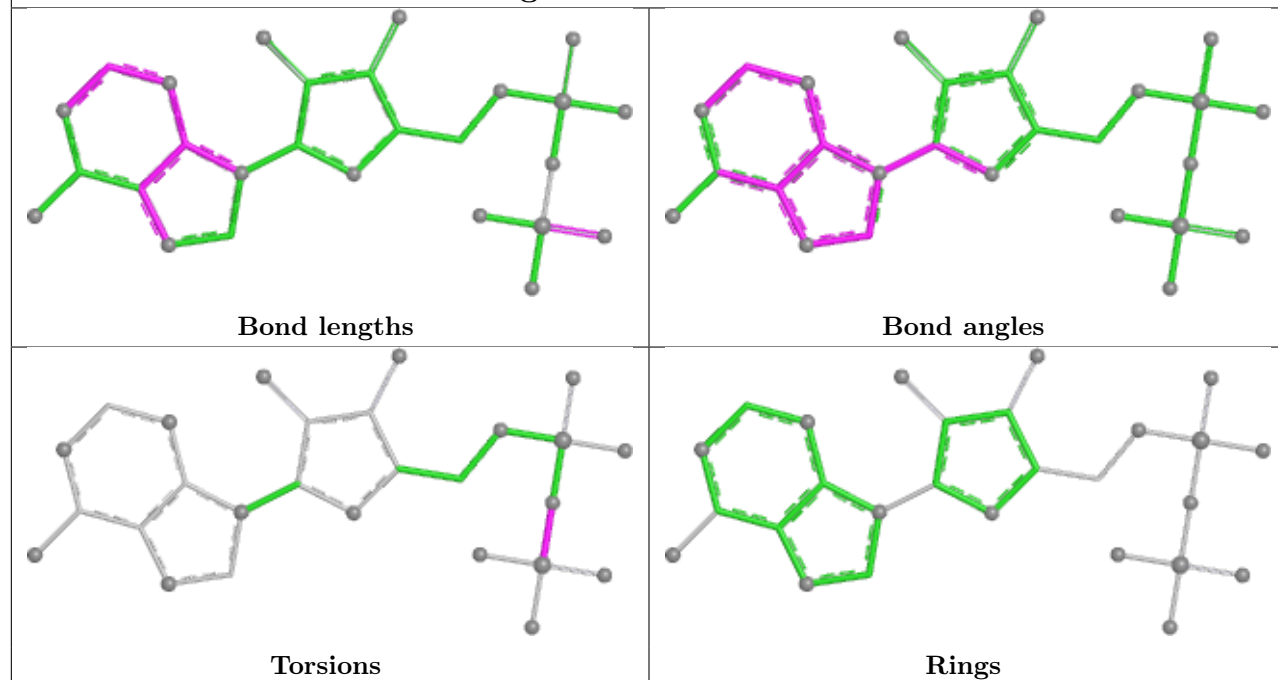
## Ligand ADP C 3528



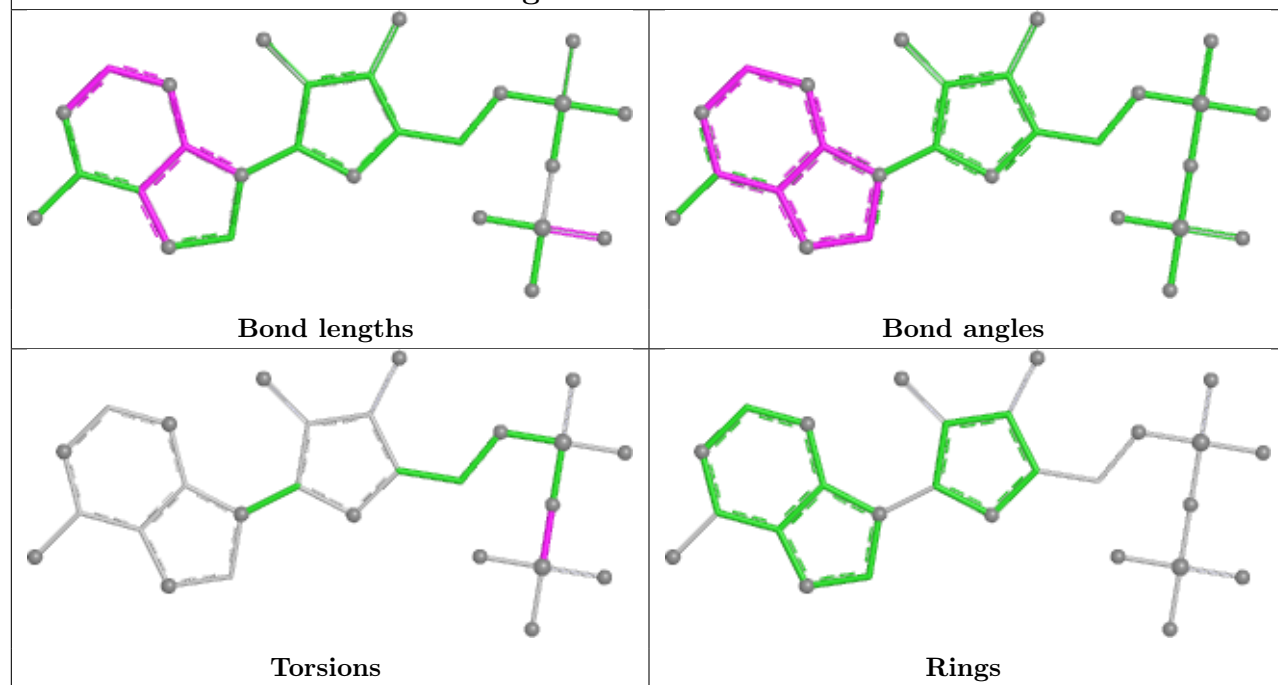
## Ligand ADP H 8528

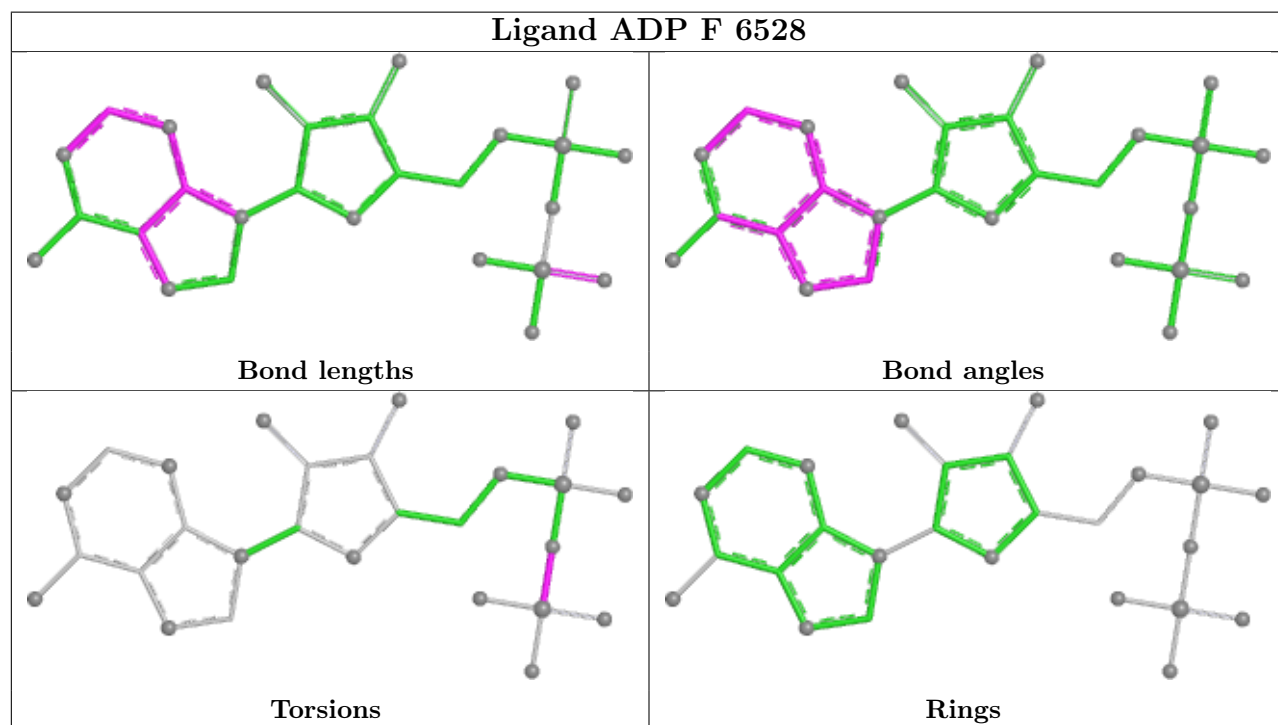
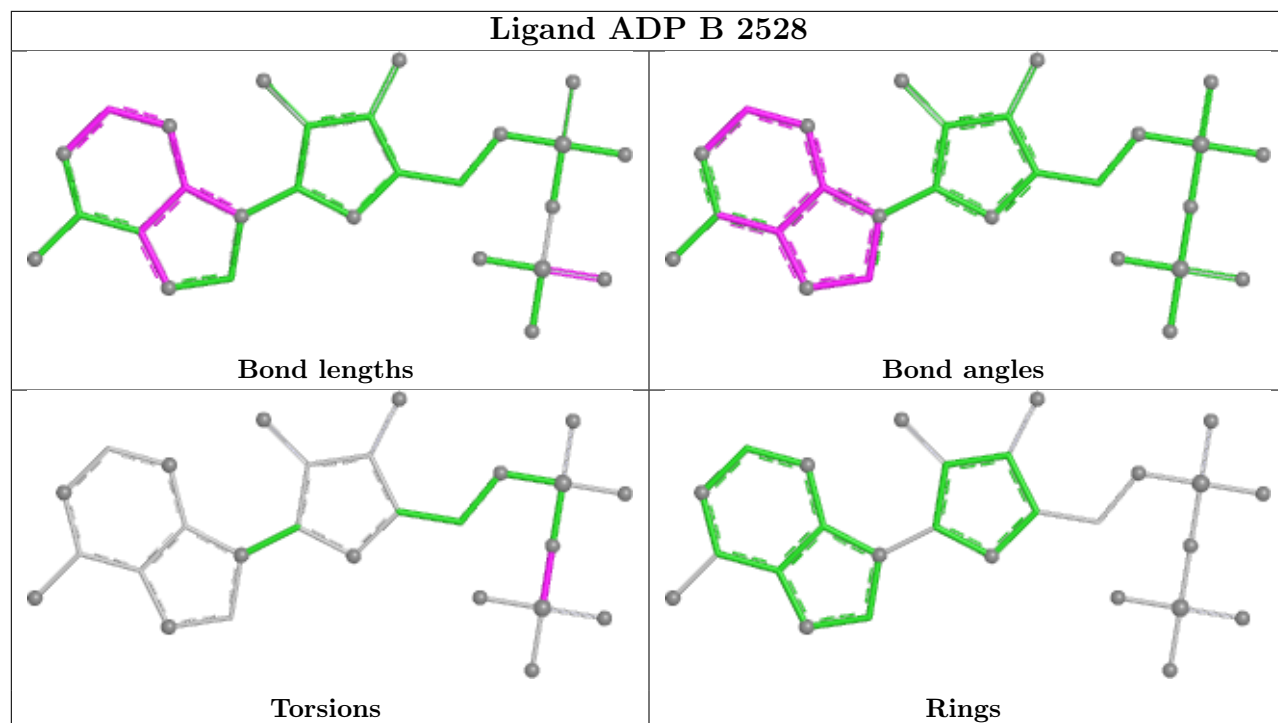


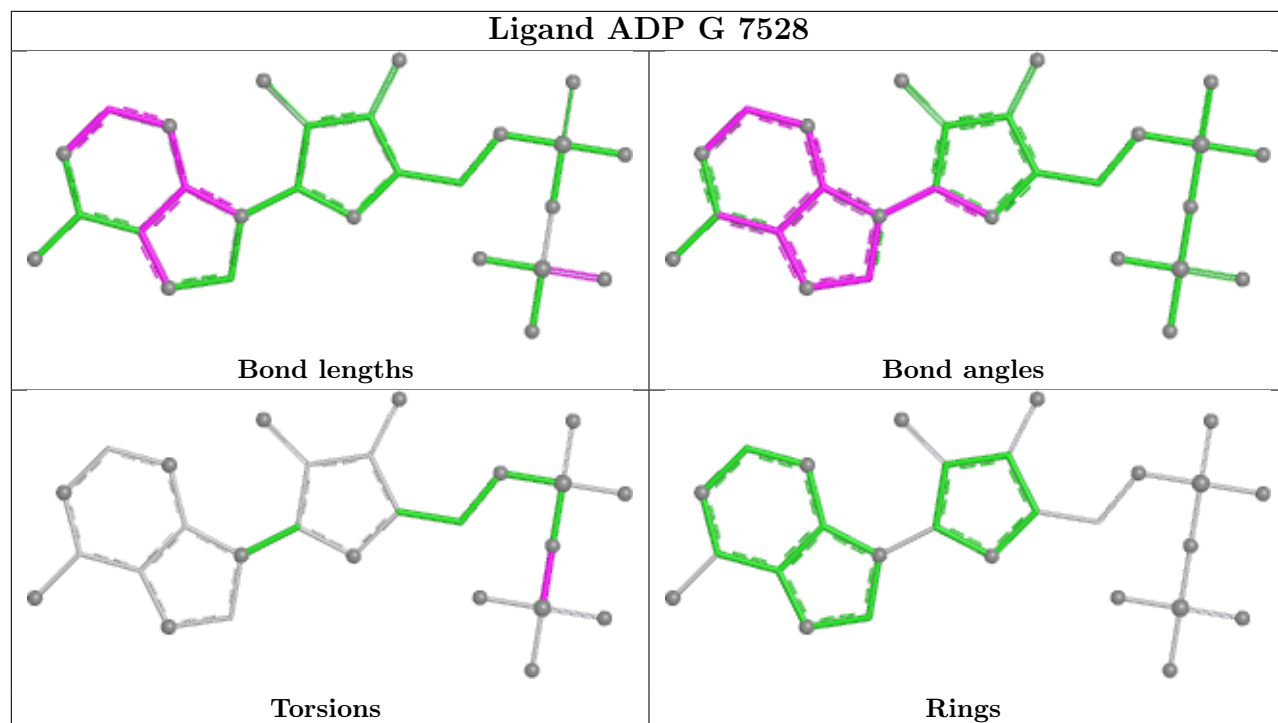
## Ligand ADP A 1528



## Ligand ADP E 5528







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 517/548 (94%)   | -0.20  | 11 (2%) 63 40 | 10, 30, 62, 102       | 0     |
| 1   | B     | 517/548 (94%)   | -0.19  | 10 (1%) 66 43 | 8, 28, 62, 105        | 0     |
| 1   | C     | 517/548 (94%)   | -0.01  | 10 (1%) 66 43 | 16, 40, 70, 100       | 0     |
| 1   | D     | 517/548 (94%)   | 0.10   | 11 (2%) 63 40 | 13, 41, 70, 102       | 0     |
| 1   | E     | 517/548 (94%)   | 0.06   | 11 (2%) 63 40 | 16, 41, 67, 108       | 0     |
| 1   | F     | 517/548 (94%)   | -0.07  | 16 (3%) 51 30 | 14, 34, 65, 109       | 0     |
| 1   | G     | 517/548 (94%)   | -0.07  | 10 (1%) 66 43 | 12, 35, 65, 98        | 0     |
| 1   | H     | 517/548 (94%)   | -0.20  | 11 (2%) 63 40 | 8, 29, 56, 96         | 0     |
| All | All   | 4136/4384 (94%) | -0.07  | 90 (2%) 62 39 | 8, 35, 66, 109        | 0     |

All (90) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 11  | ILE  | 8.0  |
| 1   | H     | 11  | ILE  | 7.5  |
| 1   | D     | 11  | ILE  | 7.2  |
| 1   | E     | 11  | ILE  | 7.2  |
| 1   | F     | 11  | ILE  | 7.2  |
| 1   | B     | 10  | VAL  | 6.9  |
| 1   | C     | 11  | ILE  | 6.2  |
| 1   | E     | 526 | ALA  | 5.9  |
| 1   | G     | 11  | ILE  | 5.7  |
| 1   | D     | 526 | ALA  | 5.7  |
| 1   | C     | 10  | VAL  | 5.5  |
| 1   | E     | 10  | VAL  | 5.5  |
| 1   | H     | 10  | VAL  | 5.4  |
| 1   | A     | 526 | ALA  | 4.8  |
| 1   | A     | 189 | LYS  | 4.8  |
| 1   | F     | 525 | LYS  | 4.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 10  | VAL  | 4.5  |
| 1   | C     | 12  | LEU  | 4.2  |
| 1   | G     | 10  | VAL  | 4.1  |
| 1   | D     | 167 | ALA  | 4.1  |
| 1   | B     | 12  | LEU  | 3.9  |
| 1   | H     | 189 | LYS  | 3.4  |
| 1   | G     | 167 | ALA  | 3.4  |
| 1   | E     | 12  | LEU  | 3.3  |
| 1   | B     | 258 | ASN  | 3.3  |
| 1   | F     | 526 | ALA  | 3.3  |
| 1   | C     | 525 | LYS  | 3.2  |
| 1   | D     | 10  | VAL  | 3.2  |
| 1   | A     | 190 | ASP  | 3.2  |
| 1   | D     | 171 | LYS  | 3.1  |
| 1   | E     | 525 | LYS  | 3.1  |
| 1   | H     | 526 | ALA  | 3.1  |
| 1   | F     | 12  | LEU  | 3.1  |
| 1   | G     | 526 | ALA  | 3.0  |
| 1   | D     | 12  | LEU  | 3.0  |
| 1   | F     | 164 | GLY  | 3.0  |
| 1   | H     | 258 | ASN  | 3.0  |
| 1   | B     | 526 | ALA  | 3.0  |
| 1   | E     | 189 | LYS  | 2.9  |
| 1   | D     | 169 | SER  | 2.8  |
| 1   | B     | 525 | LYS  | 2.8  |
| 1   | G     | 525 | LYS  | 2.8  |
| 1   | C     | 167 | ALA  | 2.8  |
| 1   | D     | 166 | ASN  | 2.8  |
| 1   | A     | 525 | LYS  | 2.8  |
| 1   | H     | 164 | GLY  | 2.7  |
| 1   | H     | 12  | LEU  | 2.7  |
| 1   | H     | 14  | GLU  | 2.7  |
| 1   | A     | 164 | GLY  | 2.7  |
| 1   | E     | 258 | ASN  | 2.7  |
| 1   | C     | 526 | ALA  | 2.7  |
| 1   | G     | 189 | LYS  | 2.6  |
| 1   | C     | 189 | LYS  | 2.6  |
| 1   | E     | 263 | ASP  | 2.6  |
| 1   | D     | 358 | GLU  | 2.6  |
| 1   | B     | 524 | ALA  | 2.6  |
| 1   | A     | 524 | ALA  | 2.5  |
| 1   | F     | 524 | ALA  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 525 | LYS  | 2.5  |
| 1   | H     | 167 | ALA  | 2.4  |
| 1   | F     | 382 | HIS  | 2.4  |
| 1   | G     | 12  | LEU  | 2.4  |
| 1   | C     | 164 | GLY  | 2.4  |
| 1   | B     | 189 | LYS  | 2.4  |
| 1   | A     | 258 | ASN  | 2.4  |
| 1   | A     | 167 | ALA  | 2.4  |
| 1   | H     | 524 | ALA  | 2.4  |
| 1   | A     | 382 | HIS  | 2.3  |
| 1   | F     | 189 | LYS  | 2.3  |
| 1   | B     | 167 | ALA  | 2.3  |
| 1   | F     | 15  | GLY  | 2.3  |
| 1   | F     | 166 | ASN  | 2.3  |
| 1   | G     | 166 | ASN  | 2.3  |
| 1   | F     | 190 | ASP  | 2.3  |
| 1   | C     | 263 | ASP  | 2.2  |
| 1   | D     | 164 | GLY  | 2.2  |
| 1   | E     | 58  | ASP  | 2.2  |
| 1   | B     | 164 | GLY  | 2.2  |
| 1   | F     | 165 | LYS  | 2.1  |
| 1   | F     | 188 | LYS  | 2.1  |
| 1   | E     | 358 | GLU  | 2.1  |
| 1   | F     | 169 | SER  | 2.1  |
| 1   | H     | 190 | ASP  | 2.1  |
| 1   | G     | 17  | GLN  | 2.1  |
| 1   | C     | 190 | ASP  | 2.1  |
| 1   | A     | 10  | VAL  | 2.0  |
| 1   | G     | 190 | ASP  | 2.0  |
| 1   | A     | 187 | GLU  | 2.0  |
| 1   | E     | 524 | ALA  | 2.0  |
| 1   | F     | 167 | ALA  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

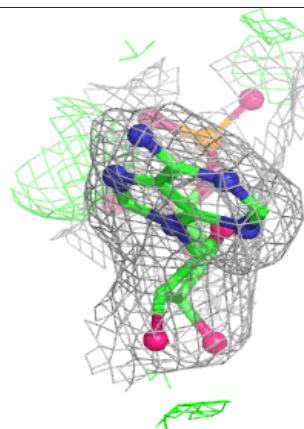
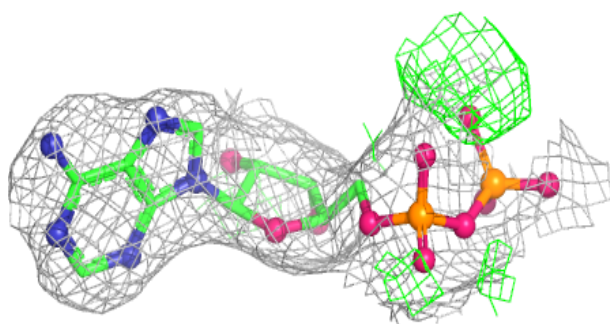
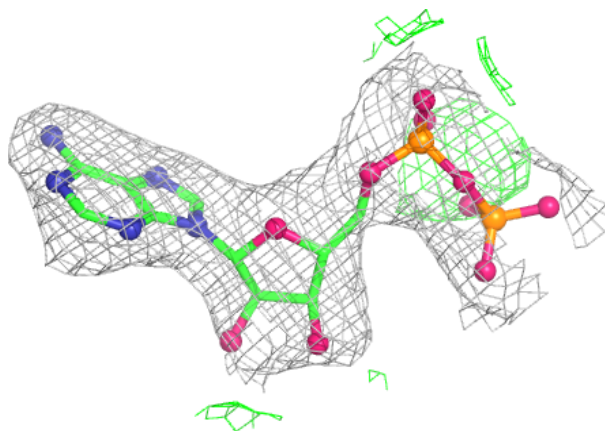
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | MG   | A     | 1527 | 1/1   | 0.87 | 0.11 | 15,15,15,15                 | 0     |
| 2   | MG   | H     | 8527 | 1/1   | 0.89 | 0.14 | 25,25,25,25                 | 0     |
| 3   | ADP  | F     | 6528 | 27/27 | 0.93 | 0.09 | 21,27,34,35                 | 0     |
| 3   | ADP  | A     | 1528 | 27/27 | 0.94 | 0.10 | 21,33,39,41                 | 0     |
| 3   | ADP  | D     | 4528 | 27/27 | 0.94 | 0.10 | 32,37,44,45                 | 0     |
| 3   | ADP  | E     | 5528 | 27/27 | 0.94 | 0.09 | 30,32,35,36                 | 0     |
| 2   | MG   | E     | 5527 | 1/1   | 0.94 | 0.13 | 14,14,14,14                 | 0     |
| 3   | ADP  | C     | 3528 | 27/27 | 0.95 | 0.09 | 32,35,37,38                 | 0     |
| 2   | MG   | C     | 3527 | 1/1   | 0.95 | 0.10 | 18,18,18,18                 | 0     |
| 2   | MG   | G     | 6527 | 1/1   | 0.95 | 0.09 | 16,16,16,16                 | 0     |
| 3   | ADP  | B     | 2528 | 27/27 | 0.95 | 0.08 | 17,24,28,29                 | 0     |
| 3   | ADP  | G     | 7528 | 27/27 | 0.95 | 0.10 | 30,39,44,45                 | 0     |
| 3   | ADP  | H     | 8528 | 27/27 | 0.95 | 0.09 | 26,28,31,32                 | 0     |
| 2   | MG   | D     | 4527 | 1/1   | 0.97 | 0.11 | 17,17,17,17                 | 0     |
| 2   | MG   | B     | 2527 | 1/1   | 0.97 | 0.15 | 10,10,10,10                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

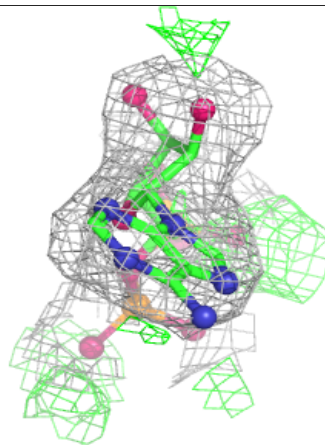
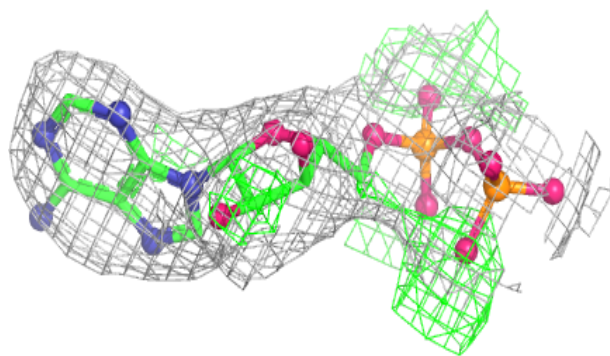
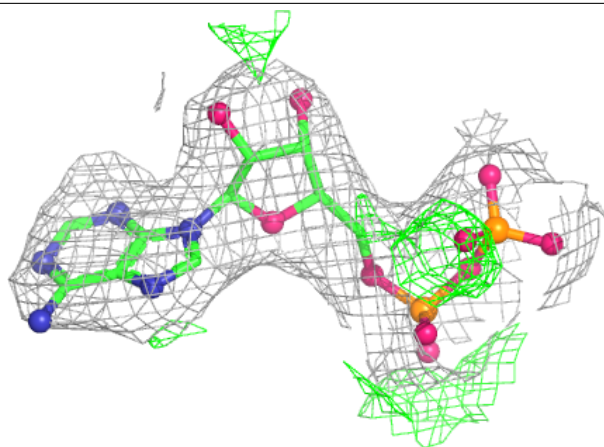
**Electron density around ADP F 6528:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



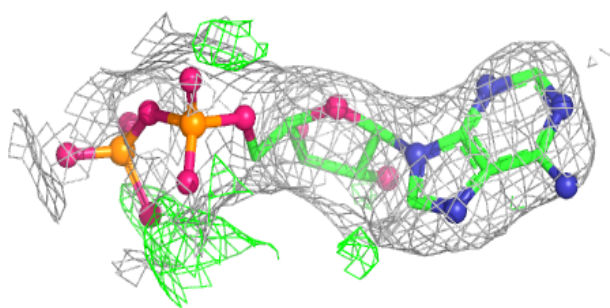
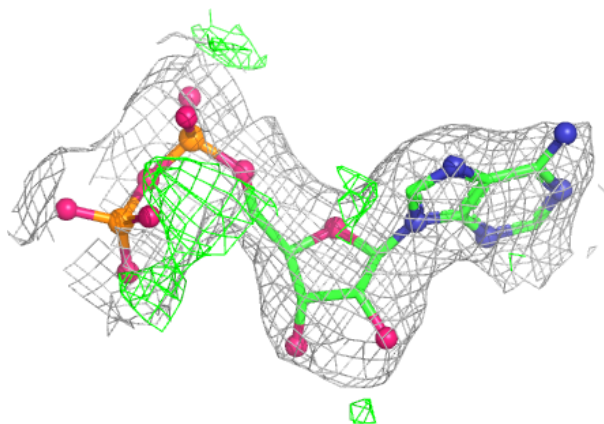
**Electron density around ADP A 1528:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

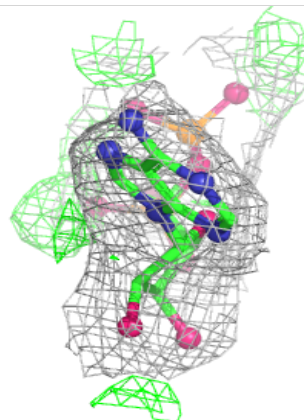
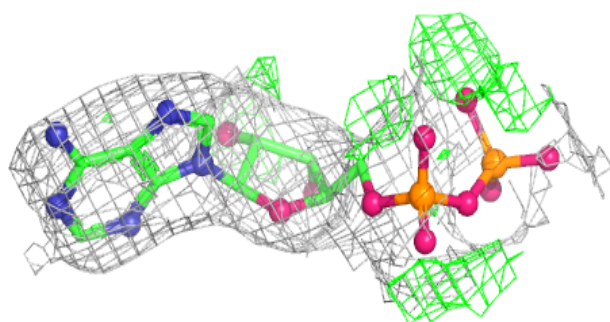
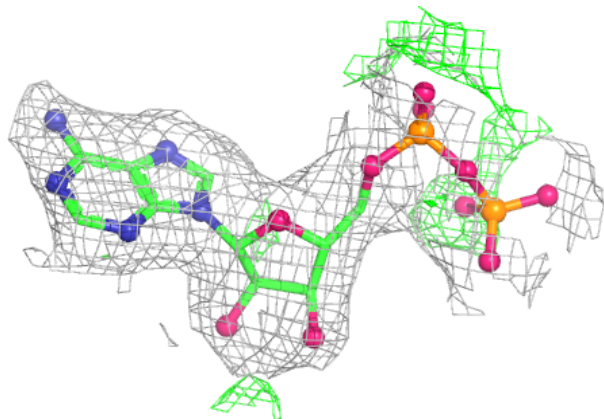


**Electron density around ADP D 4528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

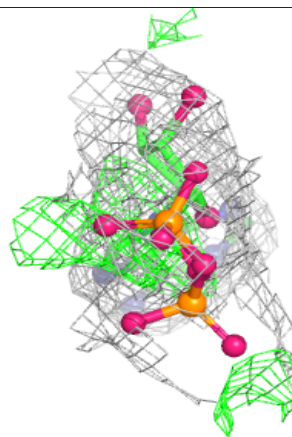
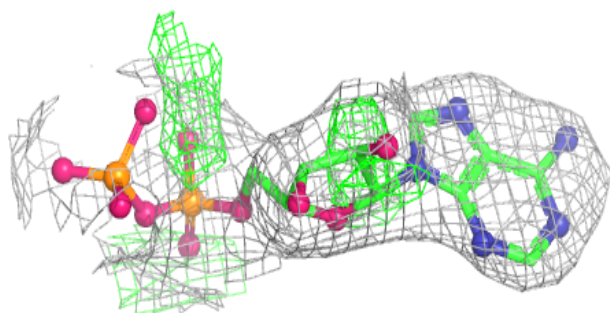
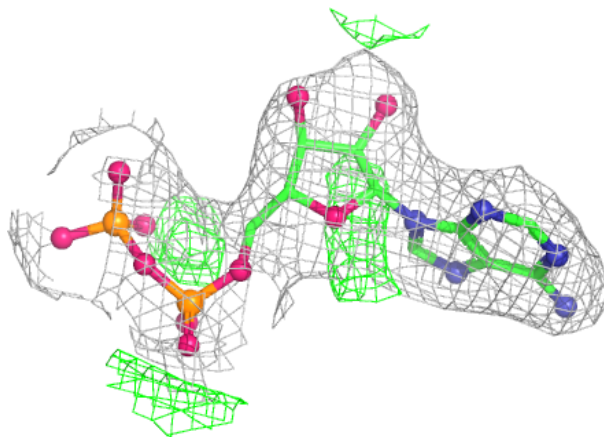
**Electron density around ADP E 5528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



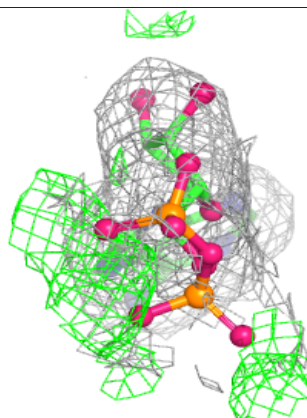
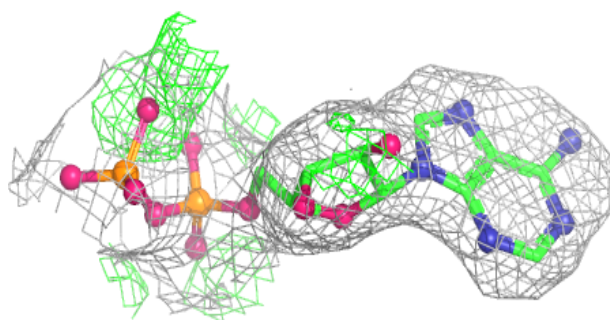
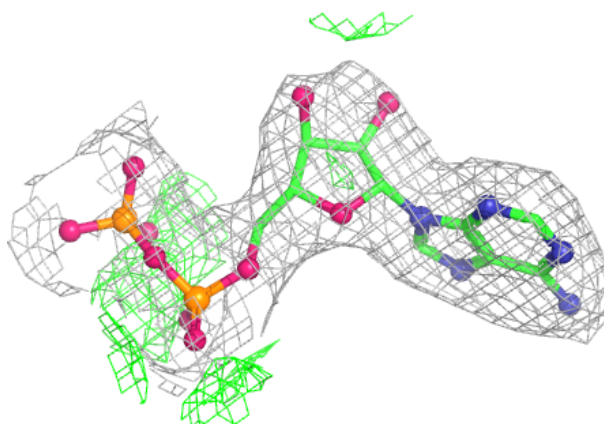
**Electron density around ADP C 3528:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

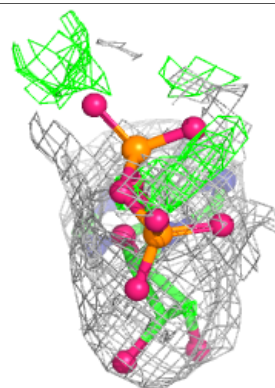
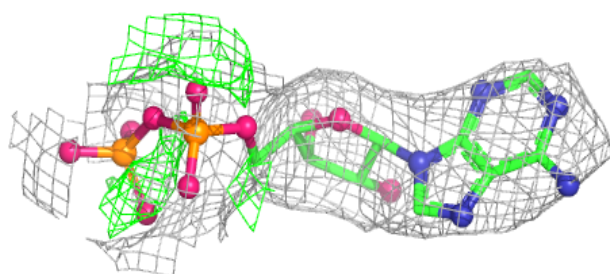
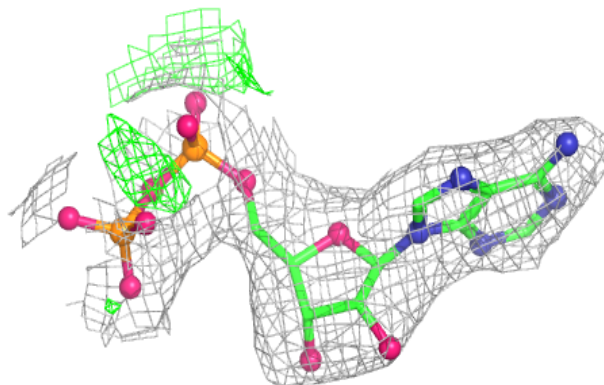


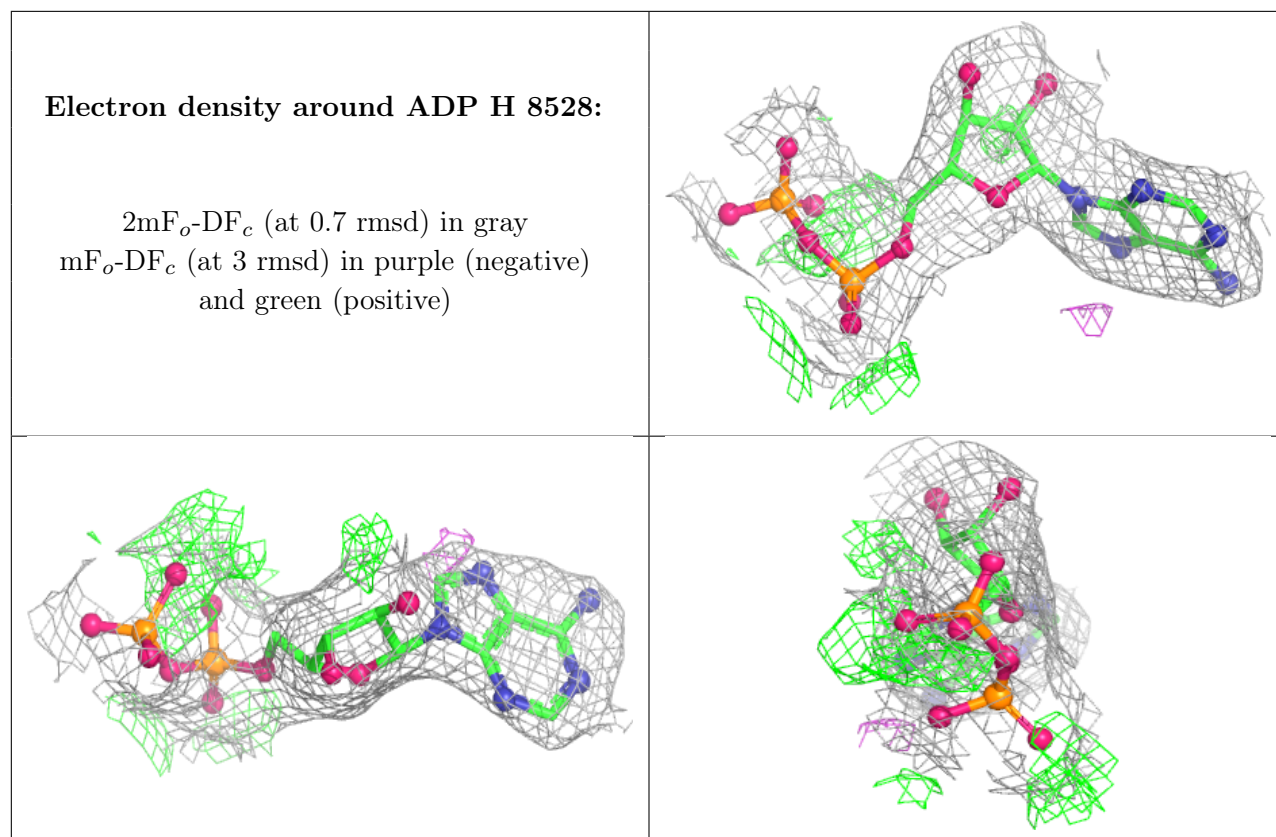
**Electron density around ADP B 2528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP G 7528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.